

# FIGURE 1

## Amino acid sequence for full-length human wild type HSD11B1 [SEQ. ID No. 1] (Residues 24-292 are underlined)

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1  MAFMKKYL LP  ILGLFMAYYY  YSANEEFRPE  MLQGKKVIVT  GASKGIGREM  AYHLAKMGAH
61  VVVTARSKET  LQKVVSHCLE  LGAASAHYIA  GTMEDMTFAE  QFVAQAGKLM  GGLDMLILNH
121 ITNTSLNLFH  DDIHHVRKSM  EVNFLSYVVL  TVAALPMLKQ  SNGSIVVVSS  LAGKVAYPMV
181 AAYSASKFAL  DGFFSSIRKE  YSVSRVNVSI  TLCVLGLIDT  ETAMKAVSGI  VHMQAAPKEE
241 CALEIIKGA   LRQEEVYYDS  SLWTTLLIRN  PCRKILEFLY  STSYNMDRFI  NK

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## Human cDNA sequence encoding residues 24-292 of HSD11B1 [SEQ. ID No. 2]

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1  AACGAGGAAT  TCAGACCAGA  GATGCTCCAA  GGAAAGAAAG  TGATTGTCAC  AGGGGCCAGC
61  AAAGGGATCG  GAAGAGAGAT  GGCTTATCAT  CTGGCGAAGA  TGGGAGCCCA  TGTGGTGGTG
121 ACAGCGAGGT  CAAAAGAAAC  TCTACAGAAG  GTGGTATCCC  ACTGCCTGGA  GCTTGGAGCA
181 GCCTCAGCAC  ACTACATTGC  TGGCACCATG  GAAGACATGA  CCTTCGCAGA  GCAATTTGTT
241 GCCCAAGCAG  GAAAGCTCAT  GGGAGGACTA  GACATGCTCA  TTCTCAACCA  CATCACCAAC
301 ACTTCTTTGA  ATCTTTTTC  TGATGATATT  CACCATGTGC  GCAAAAAGCAT  GGAAGTCAAC
361 TTCCTCAGTT  ACGTGGTCCT  GACTGTAGCT  GCCTTGCCCA  TGCTGAAGCA  GAGCAATGGA
421 AGCATTGTTG  TCGTCTCCTC  TCTGGCTGGG  AAAGTGGCTT  ATCCAATGGT  TGCTGCCTAT
481 TCTGCAAGCA  AGTTTGCTTT  GGATGGGTTC  TTCTCCTCCA  TCAGAAAGGA  ATATTCAAGT
541 TCCAGGGTCA  ATGTATCAAT  CACTCTCTGT  GTTCTTGCC  TCATAGACAC  AGAAACAGCC
601 ATGAAGGCAG  TTTCTGGGAT  AGTCCATATG  CAAGCAGCTC  CAAAGGAGGA  ATGTGCCCTG
661 GAGATCATCA  AAGGGGGAGC  TCTGCGCCAA  GAAGAAGTGT  ATTATGACAG  CTCACTCTGG
721 ACCACTCTTC  TGATCAGAAA  TCCATGCAGG  AAGATCCTGG  AATTTCTCTA  CTCAACGAGC
781 TATAATATGG  ACAGATTCAT  AAACAAG

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## Human cDNA sequence encoding residues 24-258 of HSD11B1 [SEQ. ID No. 3]

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1  AACGAGGAAT  TCAGACCAGA  GATGCTCCAA  GGAAAGAAAG  TGATTGTCAC  AGGGGCCAGC
61  AAAGGGATCG  GAAGAGAGAT  GGCTTATCAT  CTGGCGAAGA  TGGGAGCCCA  TGTGGTGGTG
121 ACAGCGAGGT  CAAAAGAAAC  TCTACAGAAG  GTGGTATCCC  ACTGCCTGGA  GCTTGGAGCA
181 GCCTCAGCAC  ACTACATTGC  TGGCACCATG  GAAGACATGA  CCTTCGCAGA  GCAATTTGTT
241 GCCCAAGCAG  GAAAGCTCAT  GGGAGGACTA  GACATGCTCA  TTCTCAACCA  CATCACCAAC
301 ACTTCTTTGA  ATCTTTTTC  TGATGATATT  CACCATGTGC  GCAAAAAGCAT  GGAAGTCAAC
361 TTCCTCAGTT  ACGTGGTCCT  GACTGTAGCT  GCCTTGCCCA  TGCTGAAGCA  GAGCAATGGA
421 AGCATTGTTG  TCGTCTCCTC  TCTGGCTGGG  AAAGTGGCTT  ATCCAATGGT  TGCTGCCTAT
481 TCTGCAAGCA  AGTTTGCTTT  GGATGGGTTC  TTCTCCTCCA  TCAGAAAGGA  ATATTCAAGT
541 TCCAGGGTCA  ATGTATCAAT  CACTCTCTGT  GTTCTTGCC  TCATAGACAC  AGAAACAGCC
601 ATGAAGGCAG  TTTCTGGGAT  AGTCCATATG  CAAGCAGCTC  CAAAGGAGGA  ATGTGCCCTG
661 GAGATCATCA  AAGGGGGAGC  TCTGCGCCAA  GAAGAAGTGT  ATTAT

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## FIGURE 1 (cont.)

### Human cDNA sequence encoding residues 24-267 of HSD11B1 [SEQ. ID No. 4]

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1 AACGAGGAAT TCAGACCAGA GATGCTCCAA GGAAAGAAAG TGATTGTCAC AGGGGCCAGC
61 AAAGGGATCG GAAGAGAGAT GGCTTATCAT CTGGCGAAGA TGGGAGCCCA TGTGGTGGTG
121 ACAGCGAGGT CAAAAGAAAC TCTACAGAAG GTGGTATCCC ACTGCCTGGA GCTTGGAGCA
181 GCCTCAGCAC ACTACATTGC TGGCACCATG GAAGACATGA CCTTCGCAGA GCAATTTGTT
241 GCCCAAGCAG GAAAGCTCAT GGGAGGACTA GACATGCTCA TTCTCAACCA CATCACCAAC
301 ACTTCTTTGA ATCTTTTTC TATGATGATATT CACCATGTGC GCAAAAGCAT GGAAGTCAAC
361 TTCCTCAGTT ACGTGGTCTT GACTGTAGCT GCCTTGCCCA TGCTGAAGCA GAGCAATGGA
421 AGCATTGTTG TCGTCTCCTC TCTGGCTGGG AAAGTGGCTT ATCCAATGGT TGCTGCCTAT
481 TCTGCAAGCA AGTTTGCTTT GGATGGGTTT TTCTCCTCCA TCAGAAAGGA ATATTCAGTG
541 TCCAGGGTCA ATGTATCAAT CACTCTCTGT GTTCTTGGCC TCATAGACAC AGAAACAGCC
601 ATGAAGGCAG TTTCTGGGAT AGTCCATATG CAAGCAGCTC CAAAGGAGGA ATGTGCCCTG
661 GAGATCATCA AAGGGGGAGC TCTGCGCCAA GAAGAAGTGT ATTATGACAG CTCACTCTGG
721 ACCACTCTTC TG
```

### Amino acid sequence for residues 24-292 of HSB11B1 with a N-terminal MKHQHQHQHQHQHQPL tag [SEQ. ID No. 5] (N-terminal MKHQHQHQHQHQHQPL tag is underlined)

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1 MKHQHQHQHQ HQHQQPLNEE FRPEMLQGKK VIVTGASKGI GREMAYHLAK MGAHVVTAR
61 SKETLQKVVS HCLELGAASA HYIAGTMEDM TFAEQFVAQA GKLMGGLDML ILNHITNTSL
121 NLFHDDIHHV RKSMEVNFLS YVVLTVAAALP MLKQSNGSIV VVSSLAGKVA YPMVAAYSAS
181 KFALDGGFFSS IRKEYSVSRV NVSITLCVLG LIDTETAMKA VSGIVHMQAA PKEECALEII
241 KGGALRQEEV YYDSSLWTTL LIRNPCRKIL EFLYSTSYNM DRFINK
```

### Amino acid sequence for residues 24-258 of HSB11B1 with a N-terminal MKHQHQHQHQHQHQPL tag [SEQ. ID No. 6] (N-terminal MKHQHQHQHQHQHQPL tag is underlined)

```
1 MKHQHQHQHQ HQHQQPLNEE FRPEMLQGKK VIVTGASKGI GREMAYHLAK MGAHVVTAR
61 SKETLQKVVS HCLELGAASA HYIAGTMEDM TFAEQFVAQA GKLMGGLDML ILNHITNTSL
121 NLFHDDIHHV RKSMEVNFLS YVVLTVAAALP MLKQSNGSIV VVSSLAGKVA YPMVAAYSAS
181 KFALDGGFFSS IRKEYSVSRV NVSITLCVLG LIDTETAMKA VSGIVHMQAA PKEECALEII
241 KGGALRQEEV YY
```

## FIGURE 1 (cont.)

**Amino acid sequence for residues 24-267 of HSB11B1 with a  
N-terminal MKHQHQHQHQHQHQPL tag [SEQ. ID No. 7]  
(N-terminal MKHQHQHQHQHQHQPL tag is underlined)**

1 MKHQHQHQHQ HQHQQPLNEE FRPEMLQGKK VIVTGASKGI GREMAYHLAK MGAHVVVITAR  
61 SKETLQKVVS HCLELGAASA HYIAGTMEDM TFAEQFVAQA GKLMGGDLML ILNHITNTSL  
121 NLFHDDIHHV RKSMEVNFLS YVVLTVAAPL MLKQSNQSVV VVSSLAGKVA YPMVAAYSAS  
181 KFALDGGFFS IRKEYSVSRV NVSITLCVLG LIDTETAMKA VSGIVHMQAA PKEECALEII  
241 KGGALRQEEV YYDSSLWTTL L

**DNA sequence encoding PCR Primer hsd1\_24-f [SEQ. ID No. 8]**

5' -AACGAGGAATTCAGACCAGAGATG-3'

**DNA sequence encoding PCR Primer hsd1\_292-r [SEQ. ID No. 9]**

5' -CTTGTTTATGAATCTGTCCATATTATAGC-3'

**DNA sequence encoding PCR Primer hsdC272Sqcf [SEQ. ID No. 10]  
(Mutation is underlined)**

5' -TCAGAAATCCATCCAGGAAGATC-3'

**DNA sequence encoding PCR Primer hsdC272Sqcr [SEQ. ID No. 11]  
(Mutation is underlined)**

5' -GATCTTCCTGGATGGATTTCTGA-3'

**DNA sequence encoding PCR Primer hsd1-258-r [SEQ. ID No. 12]**

5' -ATAATACACTTCTTCTTGGCGCAGAGC-3'

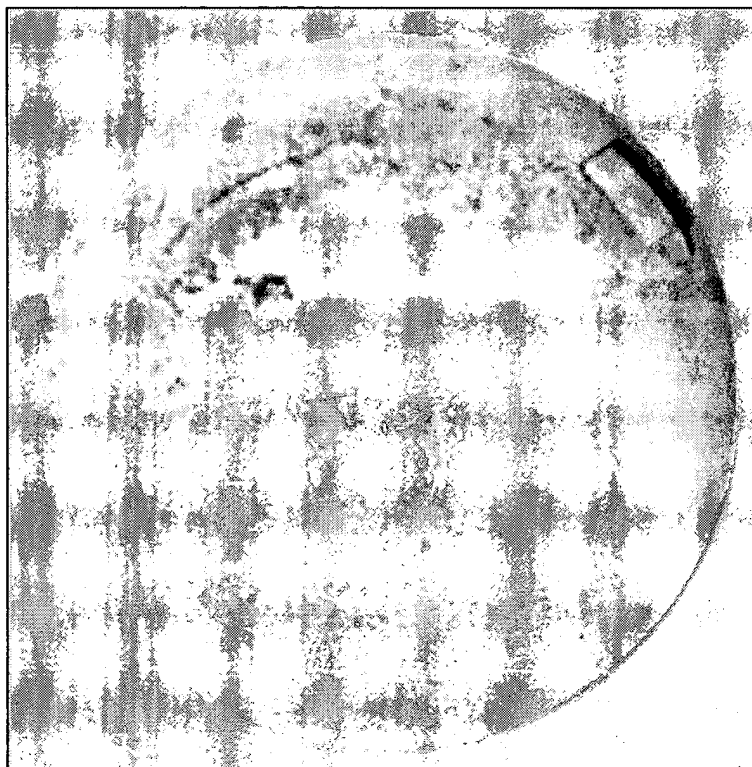
## **FIGURE 1 (cont.)**

**DNA sequence encoding PCR Primer hsd1-267-r [SEQ. ID No. 13]**

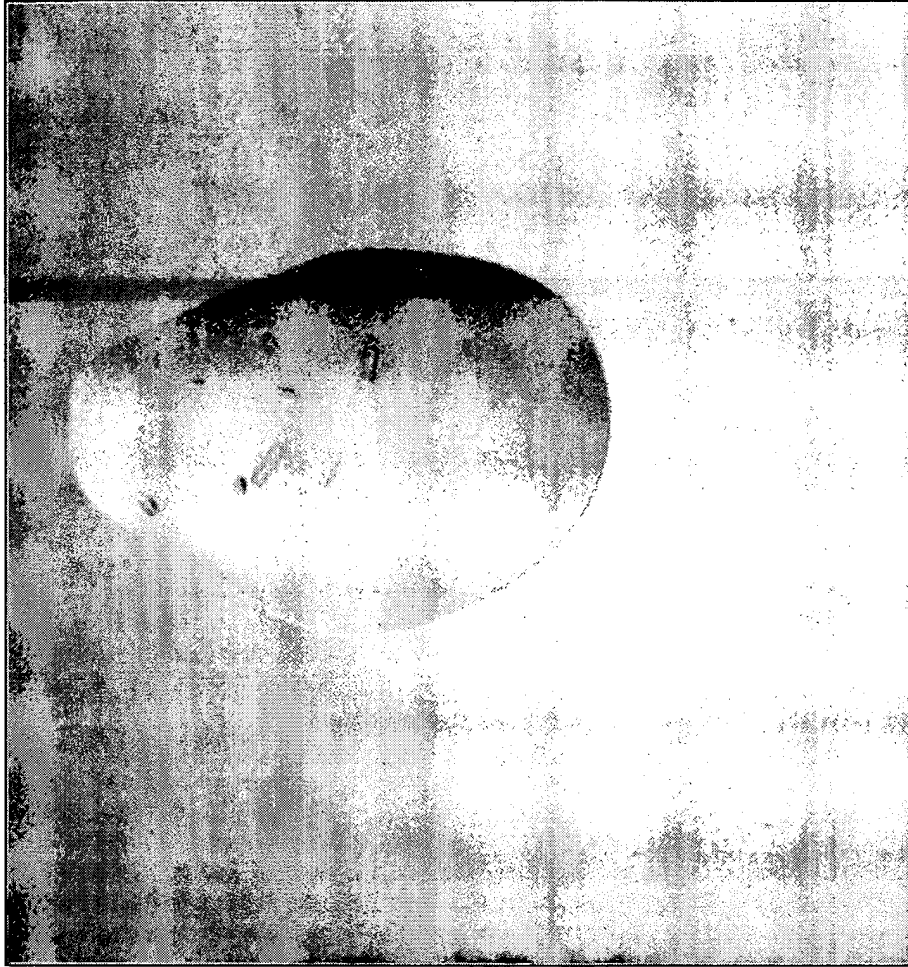
5'-CAGAAGAGTGGTCCAGAGTGAGCTGTC-3'



**FIGURE 2A**



**FIGURE 2B**



**FIGURE 2C**



# FIGURE 3

## LEGEND

Column headings from left to right are (A)'Atom Number', (B)'Atom Type', (C)'Amino Acid', (D)'Chain Identifier', (E)'Amino Acid Number', (F)'X Coordinate', (G)'Y Coordinate', (H)'Z Coordinate', (I)'Occupancy (OCC)' and (J)'B factor'.

A	B	C	D	E	F	G	H	I	J
1	N	GLN	A	21	-12.232	14.783	31.949	1.00	34.55
3	CA	GLN	A	21	-11.286	15.836	31.476	1.00	34.70
5	CB	GLN	A	21	-11.956	17.212	31.532	1.00	35.11
8	CG	GLN	A	21	-12.533	17.649	30.189	1.00	35.61
11	CD	GLN	A	21	-13.101	19.051	30.220	1.00	36.87
12	OE1	GLN	A	21	-12.372	20.017	30.461	1.00	38.31
13	NE2	GLN	A	21	-14.403	19.172	29.969	1.00	37.37
16	C	GLN	A	21	-9.970	15.838	32.268	1.00	34.48
17	O	GLN	A	21	-9.911	15.342	33.403	1.00	34.44
21	N	PRO	A	22	-8.919	16.400	31.670	1.00	34.07
22	CA	PRO	A	22	-7.573	16.317	32.244	1.00	33.86
24	CB	PRO	A	22	-6.670	16.646	31.052	1.00	33.90
27	CG	PRO	A	22	-7.479	17.534	30.194	1.00	33.94
30	CD	PRO	A	22	-8.920	17.161	30.405	1.00	34.04
33	C	PRO	A	22	-7.315	17.298	33.386	1.00	33.79
34	O	PRO	A	22	-7.820	18.426	33.379	1.00	33.70
35	N	LEU	A	23	-6.516	16.854	34.352	1.00	33.49
37	CA	LEU	A	23	-6.107	17.679	35.484	1.00	33.36
39	CB	LEU	A	23	-5.162	16.893	36.400	1.00	33.10
42	CG	LEU	A	23	-5.648	15.524	36.887	1.00	31.96
44	CD1	LEU	A	23	-4.562	14.843	37.699	1.00	31.41
48	CD2	LEU	A	23	-6.939	15.666	37.691	1.00	31.02
52	C	LEU	A	23	-5.396	18.925	34.972	1.00	33.76
53	O	LEU	A	23	-4.495	18.821	34.138	1.00	34.09
54	N	ASN	A	24	-5.806	20.095	35.461	1.00	34.10
56	CA	ASN	A	24	-5.178	21.358	35.071	1.00	34.24
58	CB	ASN	A	24	-6.202	22.502	35.048	1.00	34.53
61	CG	ASN	A	24	-7.037	22.520	33.771	1.00	35.51
62	OD1	ASN	A	24	-6.639	21.969	32.735	1.00	37.89
63	ND2	ASN	A	24	-8.199	23.159	33.838	1.00	36.53
66	C	ASN	A	24	-4.020	21.660	36.016	1.00	34.03
67	O	ASN	A	24	-4.070	22.594	36.823	1.00	34.44
68	N	GLU	A	25	-2.982	20.834	35.896	1.00	33.40
70	CA	GLU	A	25	-1.819	20.849	36.775	1.00	32.65
72	CB	GLU	A	25	-2.016	19.876	37.950	1.00	33.09
75	CG	GLU	A	25	-3.368	19.968	38.652	1.00	34.76
78	CD	GLU	A	25	-3.357	19.372	40.053	1.00	36.52
79	OE1	GLU	A	25	-3.945	19.991	40.971	1.00	38.22
80	OE2	GLU	A	25	-2.768	18.283	40.238	1.00	37.54

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
81	C	GLU	A	25	-0.590	20.414	35.984	1.00	31.40
82	O	GLU	A	25	-0.700	19.640	35.033	1.00	31.29
83	N	GLU	A	26	0.578	20.907	36.379	1.00	29.78
85	CA	GLU	A	26	1.840	20.407	35.838	1.00	28.67
87	CB	GLU	A	26	3.001	21.338	36.217	1.00	29.19
90	CG	GLU	A	26	3.969	21.624	35.075	1.00	31.46
93	CD	GLU	A	26	5.341	22.076	35.559	1.00	34.18
94	OE1	GLU	A	26	5.408	22.956	36.447	1.00	35.78
95	OE2	GLU	A	26	6.358	21.552	35.049	1.00	36.07
96	C	GLU	A	26	2.084	19.012	36.414	1.00	26.71
97	O	GLU	A	26	1.740	18.751	37.565	1.00	26.21
98	N	PHE	A	27	2.673	18.115	35.626	1.00	24.64
100	CA	PHE	A	27	3.035	16.800	36.146	1.00	23.28
102	CB	PHE	A	27	3.579	15.881	35.054	1.00	22.53
105	CG	PHE	A	27	4.011	14.541	35.573	1.00	19.85
106	CD1	PHE	A	27	3.069	13.558	35.848	1.00	18.53
108	CE1	PHE	A	27	3.459	12.318	36.343	1.00	16.99
110	CZ	PHE	A	27	4.798	12.053	36.578	1.00	17.51
112	CE2	PHE	A	27	5.751	13.028	36.312	1.00	17.43
114	CD2	PHE	A	27	5.355	14.268	35.817	1.00	19.22
116	C	PHE	A	27	4.097	16.934	37.232	1.00	23.06
117	O	PHE	A	27	5.033	17.733	37.107	1.00	22.79
118	N	ARG	A	28	3.936	16.145	38.291	1.00	22.98
120	CA	ARG	A	28	4.934	15.998	39.348	1.00	23.01
122	CB	ARG	A	28	4.439	16.647	40.643	1.00	23.40
125	CG	ARG	A	28	3.938	18.086	40.518	1.00	25.90
128	CD	ARG	A	28	3.365	18.660	41.820	1.00	28.75
131	NE	ARG	A	28	3.024	17.607	42.783	1.00	31.44
133	CZ	ARG	A	28	1.797	17.135	43.028	1.00	33.22
134	NH1	ARG	A	28	0.723	17.618	42.406	1.00	33.85
137	NH2	ARG	A	28	1.645	16.161	43.919	1.00	34.64
140	C	ARG	A	28	5.133	14.497	39.585	1.00	22.27
141	O	ARG	A	28	4.146	13.764	39.645	1.00	21.88
142	N	PRO	A	29	6.375	14.024	39.725	1.00	22.03
143	CA	PRO	A	29	6.615	12.592	39.984	1.00	21.92
145	CB	PRO	A	29	8.146	12.482	40.116	1.00	22.04
148	CG	PRO	A	29	8.687	13.864	40.124	1.00	22.46
151	CD	PRO	A	29	7.629	14.791	39.629	1.00	22.27
154	C	PRO	A	29	5.912	12.050	41.238	1.00	21.82
155	O	PRO	A	29	5.594	10.864	41.285	1.00	21.34
156	N	GLU	A	30	5.639	12.918	42.210	1.00	22.04
158	CA	GLU	A	30	4.942	12.537	43.439	1.00	21.97
160	CB	GLU	A	30	4.927	13.714	44.428	1.00	22.77
163	CG	GLU	A	30	6.284	14.045	45.032	1.00	25.13
166	CD	GLU	A	30	7.203	14.841	44.109	1.00	28.25
167	OE1	GLU	A	30	6.724	15.477	43.136	1.00	27.88
168	OE2	GLU	A	30	8.428	14.830	44.366	1.00	31.81
169	C	GLU	A	30	3.506	12.060	43.185	1.00	20.96
170	O	GLU	A	30	2.905	11.404	44.034	1.00	20.81

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
171	N	MET	A	31	2.956	12.387	42.017	1.00	20.01
173	CA	MET	A	31	1.632	11.905	41.615	1.00	19.63
175	CB	MET	A	31	1.238	12.500	40.265	1.00	19.55
178	CG	MET	A	31	0.889	13.982	40.301	1.00	20.10
181	SD	MET	A	31	0.664	14.600	38.617	1.00	20.54
182	CE	MET	A	31	-0.093	16.225	38.936	1.00	21.81
186	C	MET	A	31	1.541	10.378	41.515	1.00	19.10
187	O	MET	A	31	0.446	9.821	41.554	1.00	19.75
188	N	LEU	A	32	2.682	9.714	41.373	1.00	18.13
190	CA	LEU	A	32	2.725	8.252	41.285	1.00	17.38
192	CB	LEU	A	32	3.612	7.816	40.111	1.00	17.46
195	CG	LEU	A	32	2.980	7.731	38.720	1.00	17.94
197	CD1	LEU	A	32	2.512	9.091	38.269	1.00	18.76
201	CD2	LEU	A	32	1.841	6.724	38.688	1.00	18.52
205	C	LEU	A	32	3.219	7.576	42.567	1.00	16.75
206	O	LEU	A	32	3.230	6.351	42.659	1.00	15.57
207	N	GLN	A	33	3.646	8.362	43.552	1.00	16.57
209	CA	GLN	A	33	4.127	7.807	44.814	1.00	16.81
211	CB	GLN	A	33	4.609	8.928	45.728	1.00	17.03
214	CG	GLN	A	33	5.457	8.466	46.880	1.00	19.55
217	CD	GLN	A	33	6.117	9.637	47.587	1.00	23.05
218	OE1	GLN	A	33	7.250	9.530	48.046	1.00	27.78
219	NE2	GLN	A	33	5.408	10.754	47.669	1.00	25.68
222	C	GLN	A	33	3.028	7.014	45.513	1.00	16.02
223	O	GLN	A	33	1.937	7.522	45.745	1.00	16.34
224	N	GLY	A	34	3.311	5.752	45.806	1.00	15.47
226	CA	GLY	A	34	2.361	4.880	46.467	1.00	15.31
229	C	GLY	A	34	1.225	4.385	45.596	1.00	14.97
230	O	GLY	A	34	0.354	3.670	46.079	1.00	15.08
231	N	LYS	A	35	1.225	4.750	44.314	1.00	14.68
233	CA	LYS	A	35	0.165	4.321	43.415	1.00	14.53
235	CB	LYS	A	35	0.068	5.226	42.183	1.00	14.81
238	CG	LYS	A	35	-0.308	6.681	42.513	1.00	17.15
241	CD	LYS	A	35	-1.702	6.801	43.120	1.00	19.83
244	CE	LYS	A	35	-2.113	8.262	43.286	1.00	21.68
247	NZ	LYS	A	35	-3.354	8.403	44.107	1.00	23.59
251	C	LYS	A	35	0.396	2.877	43.010	1.00	13.89
252	O	LYS	A	35	1.526	2.409	42.973	1.00	14.09
253	N	LYS	A	36	-0.690	2.183	42.705	1.00	12.71
255	CA	LYS	A	36	-0.654	0.758	42.404	1.00	12.37
257	CB	LYS	A	36	-1.731	0.036	43.200	1.00	12.74
260	CG	LYS	A	36	-1.494	0.132	44.706	1.00	13.40
263	CD	LYS	A	36	-2.719	-0.178	45.534	1.00	15.94
266	CE	LYS	A	36	-2.455	0.188	46.986	1.00	18.33
269	NZ	LYS	A	36	-3.393	-0.468	47.929	1.00	20.06
273	C	LYS	A	36	-0.875	0.605	40.907	1.00	11.85
274	O	LYS	A	36	-1.941	0.931	40.390	1.00	11.45
275	N	VAL	A	37	0.143	0.112	40.215	1.00	11.52
277	CA	VAL	A	37	0.165	0.160	38.758	1.00	11.10

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
279	CB	VAL	A	37	1.191	1.208	38.268	1.00	11.41
281	CG1	VAL	A	37	1.122	1.363	36.747	1.00	11.58
285	CG2	VAL	A	37	0.980	2.540	38.981	1.00	11.66
289	C	VAL	A	37	0.544	-1.178	38.165	1.00	11.35
290	O	VAL	A	37	1.497	-1.799	38.614	1.00	11.33
291	N	ILE	A	38	-0.229	-1.613	37.168	1.00	10.79
293	CA	ILE	A	38	0.103	-2.755	36.327	1.00	10.52
295	CB	ILE	A	38	-1.178	-3.554	36.002	1.00	10.81
297	CG1	ILE	A	38	-1.610	-4.393	37.205	1.00	10.48
300	CD1	ILE	A	38	-2.994	-4.972	37.059	1.00	10.29
304	CG2	ILE	A	38	-0.992	-4.439	34.768	1.00	11.87
308	C	ILE	A	38	0.718	-2.251	35.031	1.00	10.89
309	O	ILE	A	38	0.208	-1.306	34.441	1.00	10.31
310	N	VAL	A	39	1.808	-2.870	34.598	1.00	10.26
312	CA	VAL	A	39	2.365	-2.610	33.270	1.00	10.58
314	CB	VAL	A	39	3.762	-1.963	33.321	1.00	10.68
316	CG1	VAL	A	39	4.175	-1.452	31.917	1.00	10.52
320	CG2	VAL	A	39	3.830	-0.856	34.332	1.00	12.19
324	C	VAL	A	39	2.491	-3.934	32.542	1.00	10.20
325	O	VAL	A	39	3.166	-4.850	33.016	1.00	10.02
326	N	THR	A	40	1.848	-4.042	31.387	1.00	10.58
328	CA	THR	A	40	2.006	-5.228	30.546	1.00	10.42
330	CB	THR	A	40	0.681	-5.670	29.887	1.00	10.70
332	OG1	THR	A	40	0.339	-4.780	28.814	1.00	11.23
334	CG2	THR	A	40	-0.487	-5.633	30.880	1.00	11.34
338	C	THR	A	40	3.080	-5.018	29.491	1.00	10.31
339	O	THR	A	40	3.491	-3.890	29.207	1.00	10.39
340	N	GLY	A	41	3.554	-6.117	28.921	1.00	10.43
342	CA	GLY	A	41	4.661	-6.046	27.984	1.00	10.23
345	C	GLY	A	41	5.852	-5.312	28.571	1.00	10.53
346	O	GLY	A	41	6.459	-4.466	27.921	1.00	10.66
347	N	ALA	A	42	6.204	-5.665	29.804	1.00	11.06
349	CA	ALA	A	42	7.131	-4.864	30.608	1.00	11.17
351	CB	ALA	A	42	6.475	-4.508	31.930	1.00	11.81
355	C	ALA	A	42	8.496	-5.503	30.837	1.00	11.69
356	O	ALA	A	42	9.270	-5.029	31.672	1.00	11.39
357	N	SER	A	43	8.823	-6.526	30.052	1.00	11.89
359	CA	SER	A	43	10.103	-7.227	30.178	1.00	12.12
361	CB	SER	A	43	9.949	-8.672	29.731	1.00	12.15
364	OG	SER	A	43	9.611	-8.763	28.365	1.00	11.52
366	C	SER	A	43	11.220	-6.549	29.384	1.00	12.17
367	O	SER	A	43	12.416	-6.793	29.619	1.00	12.38
368	N	LYS	A	44	10.820	-5.712	28.424	1.00	12.05
370	CA	LYS	A	44	11.759	-4.964	27.601	1.00	12.04
372	CB	LYS	A	44	12.334	-5.864	26.511	1.00	12.93
375	CG	LYS	A	44	11.288	-6.514	25.634	1.00	14.58
378	CD	LYS	A	44	11.886	-7.587	24.753	1.00	17.65
381	CE	LYS	A	44	10.870	-8.193	23.815	1.00	19.54
384	NZ	LYS	A	44	11.571	-9.041	22.777	1.00	20.14

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
388	C	LYS	A	44	11.046	-3.765	26.984	1.00	11.35
389	O	LYS	A	44	9.868	-3.525	27.253	1.00	11.04
390	N	GLY	A	45	11.774	-3.005	26.181	1.00	10.96
392	CA	GLY	A	45	11.202	-1.938	25.394	1.00	10.30
395	C	GLY	A	45	10.609	-0.858	26.260	1.00	9.82
396	O	GLY	A	45	11.096	-0.577	27.358	1.00	10.41
397	N	ILE	A	46	9.553	-0.233	25.754	1.00	10.01
399	CA	ILE	A	46	8.899	0.868	26.445	1.00	10.09
401	CB	ILE	A	46	7.858	1.523	25.506	1.00	10.12
403	CG1	ILE	A	46	8.563	2.073	24.248	1.00	11.19
406	CD1	ILE	A	46	7.676	2.092	22.999	1.00	12.47
410	CG2	ILE	A	46	7.070	2.616	26.245	1.00	11.56
414	C	ILE	A	46	8.270	0.437	27.767	1.00	9.79
415	O	ILE	A	46	8.339	1.162	28.738	1.00	10.38
416	N	GLY	A	47	7.681	-0.756	27.804	1.00	9.59
418	CA	GLY	A	47	7.094	-1.268	29.036	1.00	9.73
421	C	GLY	A	47	8.103	-1.361	30.163	1.00	10.00
422	O	GLY	A	47	7.810	-0.966	31.285	1.00	10.21
423	N	ARG	A	48	9.291	-1.886	29.873	1.00	10.41
425	CA	ARG	A	48	10.353	-1.953	30.876	1.00	10.68
427	CB	ARG	A	48	11.582	-2.668	30.315	1.00	10.34
430	CG	ARG	A	48	12.798	-2.614	31.216	1.00	11.49
433	CD	ARG	A	48	13.926	-3.512	30.774	1.00	12.74
436	NE	ARG	A	48	14.373	-3.169	29.432	1.00	13.41
438	CZ	ARG	A	48	15.214	-3.903	28.720	1.00	15.06
439	NH1	ARG	A	48	15.757	-5.002	29.235	1.00	17.63
442	NH2	ARG	A	48	15.550	-3.519	27.501	1.00	15.73
445	C	ARG	A	48	10.715	-0.557	31.368	1.00	10.85
446	O	ARG	A	48	10.857	-0.338	32.567	1.00	10.29
447	N	GLU	A	49	10.861	0.390	30.445	1.00	10.84
449	CA	GLU	A	49	11.181	1.761	30.823	1.00	11.07
451	CB	GLU	A	49	11.457	2.643	29.593	1.00	11.30
454	CG	GLU	A	49	12.669	2.235	28.757	1.00	14.01
457	CD	GLU	A	49	13.953	2.069	29.550	1.00	17.08
458	OE1	GLU	A	49	14.716	1.118	29.260	1.00	18.76
459	OE2	GLU	A	49	14.218	2.886	30.463	1.00	19.04
460	C	GLU	A	49	10.088	2.384	31.676	1.00	10.74
461	O	GLU	A	49	10.377	3.162	32.576	1.00	10.84
462	N	MET	A	50	8.828	2.047	31.405	1.00	9.94
464	CA	MET	A	50	7.736	2.562	32.214	1.00	10.51
466	CB	MET	A	50	6.377	2.235	31.580	1.00	10.23
469	CG	MET	A	50	6.094	3.123	30.376	1.00	11.02
472	SD	MET	A	50	4.428	3.013	29.708	1.00	12.32
473	CE	MET	A	50	4.435	1.396	28.956	1.00	11.67
477	C	MET	A	50	7.833	2.019	33.641	1.00	10.42
478	O	MET	A	50	7.681	2.770	34.587	1.00	10.58
479	N	ALA	A	51	8.104	0.722	33.773	1.00	10.80
481	CA	ALA	A	51	8.254	0.094	35.088	1.00	10.78
483	CB	ALA	A	51	8.515	-1.410	34.950	1.00	11.65



# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
487	C	ALA	A	51	9.391	0.781	35.852	1.00	10.88
488	O	ALA	A	51	9.242	1.067	37.023	1.00	11.23
489	N	TYR	A	52	10.487	1.091	35.166	1.00	11.08
491	CA	TYR	A	52	11.634	1.747	35.806	1.00	11.71
493	CB	TYR	A	52	12.854	1.742	34.881	1.00	11.74
496	CG	TYR	A	52	13.489	0.375	34.674	1.00	11.90
497	CD1	TYR	A	52	13.093	-0.740	35.429	1.00	13.42
499	CE1	TYR	A	52	13.672	-1.986	35.239	1.00	14.70
501	CZ	TYR	A	52	14.650	-2.135	34.300	1.00	14.86
502	OH	TYR	A	52	15.222	-3.383	34.128	1.00	16.48
504	CE2	TYR	A	52	15.067	-1.055	33.544	1.00	14.46
506	CD2	TYR	A	52	14.478	0.189	33.725	1.00	14.43
508	C	TYR	A	52	11.296	3.157	36.274	1.00	11.75
509	O	TYR	A	52	11.662	3.528	37.387	1.00	12.11
510	N	HIS	A	53	10.588	3.933	35.459	1.00	11.95
512	CA	HIS	A	53	10.145	5.266	35.887	1.00	11.93
514	CB	HIS	A	53	9.420	6.005	34.771	1.00	11.83
517	CG	HIS	A	53	10.335	6.612	33.755	1.00	12.67
518	ND1	HIS	A	53	11.257	7.590	34.070	1.00	14.65
520	CE1	HIS	A	53	11.902	7.948	32.972	1.00	16.59
522	NE2	HIS	A	53	11.439	7.232	31.963	1.00	15.09
524	CD2	HIS	A	53	10.463	6.384	32.427	1.00	14.67
526	C	HIS	A	53	9.219	5.195	37.095	1.00	12.21
527	O	HIS	A	53	9.378	5.963	38.041	1.00	12.17
528	N	LEU	A	54	8.255	4.280	37.055	1.00	12.00
530	CA	LEU	A	54	7.314	4.105	38.156	1.00	12.64
532	CB	LEU	A	54	6.258	3.051	37.797	1.00	12.10
535	CG	LEU	A	54	5.289	3.488	36.690	1.00	13.21
537	CD1	LEU	A	54	4.571	2.280	36.101	1.00	13.57
541	CD2	LEU	A	54	4.284	4.506	37.224	1.00	13.66
545	C	LEU	A	54	8.038	3.717	39.451	1.00	12.92
546	O	LEU	A	54	7.679	4.173	40.540	1.00	13.14
547	N	ALA	A	55	9.055	2.880	39.321	1.00	13.26
549	CA	ALA	A	55	9.860	2.432	40.442	1.00	14.00
551	CB	ALA	A	55	10.822	1.351	39.998	1.00	13.49
555	C	ALA	A	55	10.616	3.616	41.041	1.00	14.38
556	O	ALA	A	55	10.606	3.809	42.245	1.00	14.77
557	N	LYS	A	56	11.230	4.430	40.196	1.00	14.87
559	CA	LYS	A	56	11.919	5.649	40.651	1.00	15.88
561	CB	LYS	A	56	12.582	6.363	39.470	1.00	16.35
564	CG	LYS	A	56	13.856	5.709	38.953	1.00	19.70
567	CD	LYS	A	56	14.552	6.604	37.919	1.00	23.16
570	CE	LYS	A	56	15.285	5.796	36.858	1.00	25.02
573	NZ	LYS	A	56	14.361	5.036	35.976	1.00	27.17
577	C	LYS	A	56	10.957	6.617	41.372	1.00	15.91
578	O	LYS	A	56	11.357	7.323	42.303	1.00	16.11
579	N	MET	A	57	9.689	6.626	40.965	1.00	15.83
581	CA	MET	A	57	8.668	7.483	41.584	1.00	15.88
583	CB	MET	A	57	7.552	7.789	40.578	1.00	16.41

## FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
586	CG	MET	A	57	7.991	8.614	39.368	1.00	18.42
589	SD	MET	A	57	6.650	8.703	38.147	1.00	24.07
590	CE	MET	A	57	7.518	9.019	36.632	1.00	23.59
594	C	MET	A	57	8.066	6.885	42.859	1.00	15.40
595	O	MET	A	57	7.229	7.520	43.502	1.00	15.81
596	N	GLY	A	58	8.469	5.666	43.217	1.00	14.66
598	CA	GLY	A	58	7.997	5.016	44.430	1.00	13.88
601	C	GLY	A	58	6.607	4.408	44.332	1.00	13.58
602	O	GLY	A	58	5.887	4.296	45.326	1.00	13.18
603	N	ALA	A	59	6.219	4.008	43.126	1.00	13.47
605	CA	ALA	A	59	4.971	3.280	42.924	1.00	13.36
607	CB	ALA	A	59	4.545	3.362	41.460	1.00	13.40
611	C	ALA	A	59	5.097	1.813	43.347	1.00	13.24
612	O	ALA	A	59	6.200	1.278	43.489	1.00	12.97
613	N	HIS	A	60	3.952	1.187	43.590	1.00	13.02
615	CA	HIS	A	60	3.832	-0.268	43.609	1.00	12.98
617	CB	HIS	A	60	2.626	-0.690	44.448	1.00	13.48
620	CG	HIS	A	60	2.721	-0.306	45.893	1.00	14.08
621	ND1	HIS	A	60	3.332	-1.104	46.833	1.00	16.67
623	CE1	HIS	A	60	3.250	-0.525	48.020	1.00	16.27
625	NE2	HIS	A	60	2.604	0.619	47.882	1.00	16.07
627	CD2	HIS	A	60	2.256	0.776	46.561	1.00	16.82
629	C	HIS	A	60	3.603	-0.733	42.167	1.00	12.86
630	O	HIS	A	60	2.716	-0.226	41.492	1.00	12.45
631	N	VAL	A	61	4.385	-1.704	41.705	1.00	12.71
633	CA	VAL	A	61	4.287	-2.179	40.321	1.00	12.60
635	CB	BVAL	A	61	5.476	-1.744	39.410	0.35	12.73
636	CB	AVAL	A	61	5.554	-1.779	39.520	0.65	13.40
639	CG1	BVAL	A	61	5.453	-0.238	39.173	0.35	12.42
640	CG1	AVAL	A	61	5.313	-1.870	38.038	0.65	13.96
647	CG2	BVAL	A	61	6.823	-2.200	39.971	0.35	12.03
648	CG2	AVAL	A	61	6.022	-0.370	39.906	0.65	13.70
655	C	VAL	A	61	4.121	-3.697	40.240	1.00	12.53
656	O	VAL	A	61	4.782	-4.459	40.958	1.00	12.29
657	N	VAL	A	62	3.235	-4.131	39.358	1.00	11.15
659	CA	VAL	A	62	3.206	-5.520	38.934	1.00	11.52
661	CB	VAL	A	62	1.911	-6.233	39.294	1.00	11.40
663	CG1	VAL	A	62	1.906	-7.661	38.747	1.00	12.59
667	CG2	VAL	A	62	1.731	-6.241	40.797	1.00	12.96
671	C	VAL	A	62	3.424	-5.512	37.435	1.00	11.25
672	O	VAL	A	62	2.688	-4.867	36.699	1.00	12.25
673	N	VAL	A	63	4.450	-6.221	36.994	1.00	11.10
675	CA	VAL	A	63	4.777	-6.317	35.586	1.00	10.89
677	CB	VAL	A	63	6.276	-5.979	35.315	1.00	11.00
679	CG1	VAL	A	63	7.221	-6.835	36.140	1.00	11.07
683	CG2	VAL	A	63	6.522	-4.511	35.596	1.00	12.45
687	C	VAL	A	63	4.447	-7.701	35.041	1.00	10.25
688	O	VAL	A	63	4.464	-8.705	35.769	1.00	10.68
689	N	THR	A	64	4.178	-7.753	33.749	1.00	10.04

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
691	CA	THR	A	64	3.937	-9.010	33.080	1.00	10.00
693	CB	THR	A	64	2.437	-9.391	33.174	1.00	10.15
695	OG1	THR	A	64	2.204	-10.714	32.660	1.00	11.09
697	CG2	THR	A	64	1.543	-8.446	32.352	1.00	11.35
701	C	THR	A	64	4.470	-9.026	31.638	1.00	10.09
702	O	THR	A	64	4.730	-7.978	31.031	1.00	10.64
703	N	ALA	A	65	4.636	-10.257	31.163	1.00	10.16
705	CA	ALA	A	65	5.165	-10.672	29.862	1.00	10.42
707	CB	ALA	A	65	6.556	-10.118	29.610	1.00	11.04
711	C	ALA	A	65	5.197	-12.210	29.918	1.00	10.80
712	O	ALA	A	65	4.872	-12.802	30.952	1.00	10.46
713	N	ARG	A	66	5.591	-12.867	28.840	1.00	10.82
715	CA	ARG	A	66	5.682	-14.338	28.854	1.00	11.03
717	CB	ARG	A	66	5.707	-14.890	27.430	1.00	11.05
720	CG	ARG	A	66	4.372	-14.734	26.716	1.00	11.27
723	CD	ARG	A	66	4.404	-15.115	25.278	1.00	12.07
726	NE	ARG	A	66	5.361	-14.290	24.571	1.00	11.37
728	CZ	ARG	A	66	5.763	-14.509	23.336	1.00	12.92
729	NH1	ARG	A	66	6.662	-13.706	22.798	1.00	12.82
732	NH2	ARG	A	66	5.242	-15.503	22.618	1.00	14.26
735	C	ARG	A	66	6.892	-14.869	29.617	1.00	11.29
736	O	ARG	A	66	6.803	-15.915	30.257	1.00	12.14
737	N	SER	A	67	8.008	-14.149	29.570	1.00	11.42
739	CA	SER	A	67	9.293	-14.685	30.032	1.00	11.75
741	CB	BSER	A	67	10.409	-14.158	29.131	0.35	11.87
742	CB	ASER	A	67	10.453	-14.176	29.168	0.65	12.08
747	OG	BSER	A	67	10.027	-14.220	27.769	0.35	12.52
748	OG	ASER	A	67	11.720	-14.530	29.737	0.65	12.89
751	C	SER	A	67	9.585	-14.345	31.489	1.00	11.44
752	O	SER	A	67	9.877	-13.190	31.808	1.00	11.69
753	N	LYS	A	68	9.583	-15.356	32.360	1.00	11.26
755	CA	LYS	A	68	9.923	-15.139	33.771	1.00	11.27
757	CB	LYS	A	68	9.662	-16.401	34.609	1.00	11.34
760	CG	LYS	A	68	10.568	-17.594	34.335	1.00	12.53
763	CD	LYS	A	68	10.143	-18.781	35.222	1.00	13.11
766	CE	LYS	A	68	11.021	-20.016	35.001	1.00	16.27
769	NZ	LYS	A	68	10.706	-20.680	33.702	1.00	18.42
773	C	LYS	A	68	11.361	-14.650	33.951	1.00	11.49
774	O	LYS	A	68	11.639	-13.855	34.832	1.00	11.62
775	N	GLU	A	69	12.269	-15.093	33.093	1.00	11.72
777	CA	GLU	A	69	13.684	-14.765	33.248	1.00	12.60
779	CB	GLU	A	69	14.536	-15.604	32.293	1.00	12.93
782	CG	GLU	A	69	14.568	-17.098	32.602	1.00	15.40
785	CD	GLU	A	69	13.375	-17.900	32.088	1.00	17.93
786	OE1	GLU	A	69	13.265	-19.076	32.512	1.00	20.49
787	OE2	GLU	A	69	12.539	-17.393	31.286	1.00	19.00
788	C	GLU	A	69	13.942	-13.270	33.033	1.00	12.29
789	O	GLU	A	69	14.681	-12.639	33.801	1.00	12.43
790	N	THR	A	70	13.337	-12.690	31.997	1.00	12.70

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
792	CA	THR	A	70	13.512	-11.260	31.758	1.00	12.75
794	CB	THR	A	70	13.143	-10.886	30.309	1.00	12.84
796	OG1	THR	A	70	11.836	-11.368	29.989	1.00	13.41
798	CG2	THR	A	70	14.038	-11.607	29.347	1.00	14.60
802	C	THR	A	70	12.732	-10.420	32.757	1.00	12.50
803	O	THR	A	70	13.203	-9.369	33.186	1.00	12.61
804	N	LEU	A	71	11.554	-10.895	33.156	1.00	11.60
806	CA	LEU	A	71	10.765	-10.210	34.173	1.00	11.45
808	CB	LEU	A	71	9.402	-10.878	34.346	1.00	11.15
811	CG	LEU	A	71	8.397	-10.646	33.214	1.00	11.01
813	CD1	LEU	A	71	7.222	-11.628	33.327	1.00	9.87
817	CD2	LEU	A	71	7.915	-9.219	33.171	1.00	11.18
821	C	LEU	A	71	11.477	-10.162	35.534	1.00	11.37
822	O	LEU	A	71	11.360	-9.176	36.248	1.00	11.15
823	N	GLN	A	72	12.203	-11.220	35.882	1.00	10.98
825	CA	GLN	A	72	12.960	-11.254	37.134	1.00	10.60
827	CB	GLN	A	72	13.709	-12.589	37.294	1.00	11.07
830	CG	GLN	A	72	12.790	-13.743	37.730	1.00	10.55
833	CD	GLN	A	72	13.374	-15.117	37.461	1.00	11.91
834	OE1	GLN	A	72	14.606	-15.275	37.343	1.00	13.99
835	NE2	GLN	A	72	12.505	-16.120	37.368	1.00	11.52
838	C	GLN	A	72	13.945	-10.099	37.190	1.00	10.98
839	O	GLN	A	72	14.104	-9.460	38.229	1.00	11.15
840	N	LYS	A	73	14.589	-9.833	36.054	1.00	11.09
842	CA	LYS	A	73	15.587	-8.770	35.977	1.00	12.13
844	CB	LYS	A	73	16.356	-8.855	34.657	1.00	12.43
847	CG	LYS	A	73	17.224	-10.090	34.529	1.00	16.37
850	CD	LYS	A	73	17.931	-10.129	33.181	1.00	20.53
853	CE	LYS	A	73	18.880	-11.304	33.072	1.00	23.16
856	NZ	LYS	A	73	19.965	-11.013	32.093	1.00	26.57
860	C	LYS	A	73	14.947	-7.393	36.128	1.00	11.61
861	O	LYS	A	73	15.511	-6.498	36.773	1.00	11.60
862	N	VAL	A	74	13.763	-7.222	35.547	1.00	11.01
864	CA	VAL	A	74	13.026	-5.965	35.662	1.00	11.03
866	CB	VAL	A	74	11.790	-5.935	34.740	1.00	10.98
868	CG1	VAL	A	74	10.895	-4.714	35.020	1.00	11.97
872	CG2	VAL	A	74	12.228	-5.950	33.283	1.00	11.47
876	C	VAL	A	74	12.618	-5.736	37.119	1.00	11.47
877	O	VAL	A	74	12.789	-4.644	37.646	1.00	11.95
878	N	VAL	A	75	12.100	-6.768	37.774	1.00	11.13
880	CA	VAL	A	75	11.670	-6.618	39.167	1.00	11.29
882	CB	VAL	A	75	10.963	-7.887	39.686	1.00	11.21
884	CG1	VAL	A	75	9.587	-7.987	39.048	1.00	12.05
888	CG2	VAL	A	75	10.857	-7.884	41.213	1.00	12.11
892	C	VAL	A	75	12.867	-6.251	40.050	1.00	11.60
893	O	VAL	A	75	12.780	-5.349	40.866	1.00	12.45
894	N	SER	A	76	13.984	-6.941	39.879	1.00	11.86
896	CA	SER	A	76	15.142	-6.672	40.732	1.00	12.00
898	CB	BSER	A	76	16.280	-7.677	40.495	0.35	11.95

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
899	CB	ASER	A	76	16.273	-7.656	40.417	0.65	11.99
904	OG	BSER	A	76	16.798	-7.610	39.181	0.35	12.85
905	OG	ASER	A	76	17.471	-7.307	41.083	0.65	13.95
908	C	SER	A	76	15.611	-5.227	40.555	1.00	11.96
909	O	SER	A	76	15.910	-4.549	41.544	1.00	12.62
910	N	HIS	A	77	15.658	-4.741	39.315	1.00	12.03
912	CA	HIS	A	77	16.065	-3.356	39.071	1.00	12.50
914	CB	HIS	A	77	16.358	-3.081	37.592	1.00	12.58
917	CG	HIS	A	77	17.169	-1.840	37.378	1.00	13.91
918	ND1	HIS	A	77	16.723	-0.767	36.639	1.00	17.25
920	CE1	HIS	A	77	17.642	0.183	36.646	1.00	15.02
922	NE2	HIS	A	77	18.662	-0.230	37.370	1.00	18.45
924	CD2	HIS	A	77	18.391	-1.490	37.846	1.00	15.70
926	C	HIS	A	77	15.030	-2.362	39.603	1.00	12.87
927	O	HIS	A	77	15.392	-1.303	40.108	1.00	12.83
928	N	CYS	A	78	13.742	-2.704	39.513	1.00	12.49
930	CA	CYS	A	78	12.700	-1.831	40.057	1.00	13.15
932	CB	CYS	A	78	11.298	-2.379	39.797	1.00	13.29
935	SG	CYS	A	78	10.711	-2.122	38.109	1.00	13.56
936	C	CYS	A	78	12.897	-1.623	41.553	1.00	13.28
937	O	CYS	A	78	12.791	-0.511	42.044	1.00	14.09
938	N	LEU	A	79	13.218	-2.691	42.270	1.00	14.18
940	CA	LEU	A	79	13.446	-2.596	43.710	1.00	14.52
942	CB	LEU	A	79	13.615	-3.987	44.334	1.00	14.79
945	CG	LEU	A	79	12.357	-4.860	44.310	1.00	14.95
947	CD1	LEU	A	79	11.252	-4.252	45.167	1.00	15.22
951	CD2	LEU	A	79	12.641	-6.279	44.769	1.00	16.43
955	C	LEU	A	79	14.654	-1.705	44.000	1.00	15.07
956	O	LEU	A	79	14.601	-0.870	44.900	1.00	15.81
957	N	GLU	A	80	15.723	-1.866	43.221	1.00	15.55
959	CA	GLU	A	80	16.935	-1.047	43.386	1.00	16.56
961	CB	GLU	A	80	18.011	-1.450	42.380	1.00	17.26
964	CG	GLU	A	80	18.625	-2.810	42.629	1.00	20.78
967	CD	GLU	A	80	19.649	-3.182	41.576	1.00	24.94
968	OE1	GLU	A	80	19.496	-2.760	40.403	1.00	28.44
969	OE2	GLU	A	80	20.605	-3.904	41.912	1.00	28.97
970	C	GLU	A	80	16.656	0.427	43.184	1.00	16.04
971	O	GLU	A	80	17.267	1.271	43.833	1.00	16.11
972	N	LEU	A	81	15.758	0.727	42.250	1.00	15.33
974	CA	LEU	A	81	15.416	2.098	41.885	1.00	15.28
976	CB	LEU	A	81	14.747	2.133	40.505	1.00	15.44
979	CG	LEU	A	81	15.650	1.925	39.291	1.00	15.54
981	CD1	LEU	A	81	14.792	1.810	38.042	1.00	16.22
985	CD2	LEU	A	81	16.648	3.073	39.142	1.00	16.85
989	C	LEU	A	81	14.503	2.776	42.902	1.00	15.16
990	O	LEU	A	81	14.324	3.986	42.837	1.00	16.04
991	N	GLY	A	82	13.913	1.996	43.808	1.00	14.81
993	CA	GLY	A	82	13.121	2.526	44.906	1.00	14.83
996	C	GLY	A	82	11.621	2.302	44.839	1.00	14.21

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
997	O	GLY	A	82	10.860	3.018	45.502	1.00	14.46
998	N	ALA	A	83	11.181	1.298	44.080	1.00	14.08
1000	CA	ALA	A	83	9.769	0.937	44.043	1.00	13.64
1002	CB	ALA	A	83	9.555	-0.264	43.159	1.00	13.43
1006	C	ALA	A	83	9.281	0.622	45.447	1.00	13.43
1007	O	ALA	A	83	10.009	0.008	46.239	1.00	13.84
1008	N	ALA	A	84	8.061	1.049	45.754	1.00	13.78
1010	CA	ALA	A	84	7.405	0.686	47.012	1.00	13.71
1012	CB	ALA	A	84	6.060	1.361	47.116	1.00	13.87
1016	C	ALA	A	84	7.269	-0.835	47.109	1.00	14.03
1017	O	ALA	A	84	7.489	-1.426	48.166	1.00	14.84
1018	N	SER	A	85	6.909	-1.453	45.988	1.00	13.29
1020	CA	SER	A	85	7.021	-2.893	45.800	1.00	13.20
1022	CB	SER	A	85	5.827	-3.645	46.390	1.00	13.35
1025	OG	SER	A	85	4.598	-3.252	45.790	1.00	14.56
1027	C	SER	A	85	7.109	-3.168	44.307	1.00	12.37
1028	O	SER	A	85	6.757	-2.323	43.489	1.00	12.68
1029	N	ALA	A	86	7.600	-4.352	43.969	1.00	12.05
1031	CA	ALA	A	86	7.664	-4.793	42.583	1.00	12.00
1033	CB	ALA	A	86	8.940	-4.323	41.942	1.00	11.85
1037	C	ALA	A	86	7.564	-6.311	42.523	1.00	11.93
1038	O	ALA	A	86	8.251	-7.028	43.259	1.00	12.29
1039	N	HIS	A	87	6.722	-6.790	41.621	1.00	11.65
1041	CA	HIS	A	87	6.483	-8.207	41.437	1.00	11.60
1043	CB	HIS	A	87	5.317	-8.692	42.313	1.00	12.09
1046	CG	HIS	A	87	5.554	-8.517	43.785	1.00	13.44
1047	ND1	HIS	A	87	6.340	-9.377	44.524	1.00	17.92
1049	CE1	HIS	A	87	6.388	-8.957	45.776	1.00	16.57
1051	NE2	HIS	A	87	5.660	-7.861	45.879	1.00	17.01
1053	CD2	HIS	A	87	5.137	-7.557	44.645	1.00	14.10
1055	C	HIS	A	87	6.164	-8.471	39.977	1.00	11.09
1056	O	HIS	A	87	5.713	-7.570	39.268	1.00	11.49
1057	N	TYR	A	88	6.392	-9.701	39.535	1.00	10.73
1059	CA	TYR	A	88	5.947	-10.132	38.215	1.00	10.46
1061	CB	TYR	A	88	7.133	-10.492	37.306	1.00	10.59
1064	CG	TYR	A	88	7.764	-11.840	37.554	1.00	9.92
1065	CD1	TYR	A	88	7.255	-13.001	36.974	1.00	9.00
1067	CE1	TYR	A	88	7.854	-14.244	37.205	1.00	9.09
1069	CZ	TYR	A	88	8.965	-14.312	38.018	1.00	9.49
1070	OH	TYR	A	88	9.579	-15.516	38.278	1.00	9.96
1072	CE2	TYR	A	88	9.481	-13.156	38.600	1.00	9.29
1074	CD2	TYR	A	88	8.883	-11.947	38.364	1.00	9.22
1076	C	TYR	A	88	4.990	-11.304	38.303	1.00	10.75
1077	O	TYR	A	88	5.003	-12.078	39.263	1.00	11.28
1078	N	ILE	A	89	4.164	-11.424	37.268	1.00	10.68
1080	CA	ILE	A	89	3.364	-12.611	36.995	1.00	10.79
1082	CB	ILE	A	89	1.885	-12.382	37.341	1.00	10.72
1084	CG1	ILE	A	89	1.714	-11.935	38.800	1.00	11.92
1087	CD1	ILE	A	89	0.302	-11.432	39.127	1.00	13.15

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
1091	CG2	ILE	A	89	1.074	-13.641	37.062	1.00	9.95
1095	C	ILE	A	89	3.525	-12.875	35.493	1.00	10.85
1096	O	ILE	A	89	3.233	-12.000	34.673	1.00	11.61
1097	N	ALA	A	90	4.023	-14.051	35.140	1.00	10.55
1099	CA	ALA	A	90	4.302	-14.397	33.742	1.00	10.70
1101	CB	ALA	A	90	5.570	-15.207	33.639	1.00	10.74
1105	C	ALA	A	90	3.147	-15.176	33.120	1.00	11.23
1106	O	ALA	A	90	2.527	-16.038	33.765	1.00	12.05
1107	N	GLY	A	91	2.887	-14.889	31.851	1.00	10.85
1109	CA	GLY	A	91	1.882	-15.600	31.082	1.00	10.47
1112	C	GLY	A	91	1.696	-14.986	29.712	1.00	10.22
1113	O	GLY	A	91	2.231	-13.917	29.428	1.00	9.99
1114	N	THR	A	92	0.936	-15.669	28.866	1.00	9.93
1116	CA	THR	A	92	0.657	-15.178	27.526	1.00	10.41
1118	CB	THR	A	92	0.827	-16.257	26.455	1.00	10.56
1120	OG1	THR	A	92	0.475	-15.684	25.182	1.00	11.31
1122	CG2	THR	A	92	-0.159	-17.429	26.633	1.00	10.99
1126	C	THR	A	92	-0.730	-14.560	27.442	1.00	10.36
1127	O	THR	A	92	-1.737	-15.120	27.916	1.00	10.23
1128	N	MET	A	93	-0.779	-13.395	26.816	1.00	10.51
1130	CA	MET	A	93	-2.038	-12.683	26.609	1.00	11.22
1132	CB	MET	A	93	-1.800	-11.185	26.500	1.00	11.80
1135	CG	MET	A	93	-1.251	-10.588	27.779	1.00	11.98
1138	SD	MET	A	93	-2.484	-10.548	29.090	1.00	12.19
1139	CE	MET	A	93	-1.541	-9.735	30.364	1.00	14.00
1143	C	MET	A	93	-2.826	-13.224	25.417	1.00	11.82
1144	O	MET	A	93	-3.869	-12.679	25.063	1.00	12.97
1145	N	GLU	A	94	-2.353	-14.320	24.837	1.00	11.81
1147	CA	GLU	A	94	-3.161	-15.153	23.946	1.00	12.85
1149	CB	GLU	A	94	-2.281	-16.196	23.228	1.00	13.18
1152	CG	GLU	A	94	-1.299	-15.621	22.209	1.00	16.19
1155	CD	GLU	A	94	-0.479	-16.681	21.469	1.00	21.92
1156	OE1	GLU	A	94	-0.925	-17.841	21.384	1.00	24.75
1157	OE2	GLU	A	94	0.625	-16.358	20.958	1.00	25.43
1158	C	GLU	A	94	-4.259	-15.887	24.727	1.00	13.03
1159	O	GLU	A	94	-5.275	-16.278	24.154	1.00	14.15
1160	N	ASP	A	95	-4.031	-16.074	26.029	1.00	12.98
1162	CA	ASP	A	95	-4.912	-16.836	26.919	1.00	13.19
1164	CB	ASP	A	95	-4.048	-17.699	27.839	1.00	13.08
1167	CG	ASP	A	95	-4.842	-18.496	28.843	1.00	15.34
1168	OD1	ASP	A	95	-6.065	-18.292	28.968	1.00	18.18
1169	OD2	ASP	A	95	-4.306	-19.369	29.550	1.00	17.42
1170	C	ASP	A	95	-5.754	-15.842	27.710	1.00	12.94
1171	O	ASP	A	95	-5.253	-15.184	28.610	1.00	13.26
1172	N	MET	A	96	-7.025	-15.715	27.345	1.00	13.06
1174	CA	MET	A	96	-7.905	-14.734	27.979	1.00	13.39
1176	CB	MET	A	96	-9.220	-14.608	27.206	1.00	13.93
1179	CG	MET	A	96	-9.088	-14.107	25.752	1.00	14.60
1182	SD	MET	A	96	-8.169	-12.588	25.540	1.00	17.02

## FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
1183	CE	MET	A	96	-7.076	-12.983	24.190	1.00	17.40
1187	C	MET	A	96	-8.175	-15.068	29.450	1.00	13.40
1188	O	MET	A	96	-8.461	-14.179	30.261	1.00	13.30
1189	N	THR	A	97	-8.098	-16.347	29.796	1.00	13.67
1191	CA	THR	A	97	-8.214	-16.758	31.190	1.00	13.83
1193	CB	THR	A	97	-8.342	-18.289	31.281	1.00	14.66
1195	OG1	THR	A	97	-9.548	-18.697	30.624	1.00	16.10
1197	CG2	THR	A	97	-8.507	-18.739	32.722	1.00	16.08
1201	C	THR	A	97	-7.034	-16.256	32.008	1.00	13.48
1202	O	THR	A	97	-7.203	-15.772	33.126	1.00	13.67
1203	N	PHE	A	98	-5.827	-16.355	31.459	1.00	12.78
1205	CA	PHE	A	98	-4.686	-15.751	32.114	1.00	12.66
1207	CB	PHE	A	98	-3.372	-16.021	31.371	1.00	12.69
1210	CG	PHE	A	98	-2.231	-15.214	31.917	1.00	12.56
1211	CD1	PHE	A	98	-1.638	-15.563	33.122	1.00	12.44
1213	CE1	PHE	A	98	-0.633	-14.794	33.661	1.00	13.10
1215	CZ	PHE	A	98	-0.203	-13.655	33.005	1.00	12.78
1217	CE2	PHE	A	98	-0.793	-13.286	31.815	1.00	11.98
1219	CD2	PHE	A	98	-1.812	-14.061	31.281	1.00	12.33
1221	C	PHE	A	98	-4.877	-14.243	32.300	1.00	12.89
1222	O	PHE	A	98	-4.621	-13.719	33.380	1.00	13.16
1223	N	ALA	A	99	-5.323	-13.539	31.259	1.00	12.45
1225	CA	ALA	A	99	-5.505	-12.094	31.345	1.00	12.51
1227	CB	ALA	A	99	-6.081	-11.565	30.050	1.00	12.81
1231	C	ALA	A	99	-6.400	-11.728	32.521	1.00	13.01
1232	O	ALA	A	99	-6.059	-10.866	33.329	1.00	12.89
1233	N	GLU	A	100	-7.536	-12.405	32.614	1.00	13.24
1235	CA	GLU	A	100	-8.514	-12.154	33.682	1.00	14.37
1237	CB	GLU	A	100	-9.741	-13.027	33.442	1.00	15.48
1240	CG	GLU	A	100	-10.888	-12.773	34.399	1.00	18.83
1243	CD	GLU	A	100	-12.142	-13.545	34.029	1.00	23.35
1244	OE1	GLU	A	100	-13.227	-13.169	34.534	1.00	29.89
1245	OE2	GLU	A	100	-12.051	-14.535	33.250	1.00	27.70
1246	C	GLU	A	100	-7.939	-12.455	35.072	1.00	14.40
1247	O	GLU	A	100	-8.068	-11.653	36.012	1.00	14.51
1248	N	GLN	A	101	-7.277	-13.601	35.192	1.00	13.99
1250	CA	GLN	A	101	-6.755	-14.052	36.482	1.00	13.85
1252	CB	GLN	A	101	-6.368	-15.528	36.411	1.00	14.54
1255	CG	GLN	A	101	-7.578	-16.445	36.262	1.00	16.77
1258	CD	GLN	A	101	-7.210	-17.912	36.220	1.00	19.86
1259	OE1	GLN	A	101	-6.037	-18.267	36.075	1.00	23.22
1260	NE2	GLN	A	101	-8.213	-18.770	36.342	1.00	22.94
1263	C	GLN	A	101	-5.571	-13.202	36.921	1.00	12.95
1264	O	GLN	A	101	-5.389	-12.942	38.107	1.00	12.65
1265	N	PHE	A	102	-4.782	-12.759	35.952	1.00	11.29
1267	CA	PHE	A	102	-3.635	-11.890	36.205	1.00	11.14
1269	CB	PHE	A	102	-2.900	-11.561	34.893	1.00	10.88
1272	CG	PHE	A	102	-1.997	-10.370	34.992	1.00	11.18
1273	CD1	PHE	A	102	-0.815	-10.444	35.699	1.00	11.95



# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
1275	CE1	PHE	A	102	0.004	-9.334	35.825	1.00	12.28
1277	CZ	PHE	A	102	-0.368	-8.135	35.234	1.00	12.23
1279	CE2	PHE	A	102	-1.540	-8.057	34.527	1.00	12.61
1281	CD2	PHE	A	102	-2.350	-9.165	34.406	1.00	11.71
1283	C	PHE	A	102	-4.054	-10.597	36.896	1.00	11.08
1284	O	PHE	A	102	-3.465	-10.201	37.883	1.00	10.92
1285	N	VAL	A	103	-5.054	-9.912	36.359	1.00	11.35
1287	CA	VAL	A	103	-5.486	-8.654	36.972	1.00	11.51
1289	CB	VAL	A	103	-6.579	-7.966	36.126	1.00	12.22
1291	CG1	VAL	A	103	-7.225	-6.809	36.874	1.00	12.63
1295	CG2	VAL	A	103	-5.992	-7.486	34.820	1.00	12.03
1299	C	VAL	A	103	-5.993	-8.864	38.394	1.00	11.31
1300	O	VAL	A	103	-5.670	-8.087	39.280	1.00	11.15
1301	N	ALA	A	104	-6.777	-9.914	38.608	1.00	11.51
1303	CA	ALA	A	104	-7.302	-10.215	39.939	1.00	11.36
1305	CB	ALA	A	104	-8.237	-11.427	39.888	1.00	11.80
1309	C	ALA	A	104	-6.155	-10.454	40.918	1.00	11.39
1310	O	ALA	A	104	-6.152	-9.944	42.050	1.00	11.48
1311	N	GLN	A	105	-5.180	-11.236	40.480	1.00	11.24
1313	CA	GLN	A	105	-4.032	-11.570	41.313	1.00	11.16
1315	CB	GLN	A	105	-3.162	-12.626	40.607	1.00	11.09
1318	CG	GLN	A	105	-2.058	-13.218	41.485	1.00	11.80
1321	CD	GLN	A	105	-1.302	-14.363	40.816	1.00	13.24
1322	OE1	GLN	A	105	-0.073	-14.480	40.961	1.00	15.47
1323	NE2	GLN	A	105	-2.023	-15.214	40.112	1.00	12.86
1326	C	GLN	A	105	-3.201	-10.333	41.639	1.00	11.06
1327	O	GLN	A	105	-2.813	-10.115	42.783	1.00	11.09
1328	N	ALA	A	106	-2.896	-9.535	40.614	1.00	10.33
1330	CA	ALA	A	106	-2.081	-8.338	40.779	1.00	10.58
1332	CB	ALA	A	106	-1.789	-7.689	39.415	1.00	11.01
1336	C	ALA	A	106	-2.743	-7.337	41.719	1.00	10.76
1337	O	ALA	A	106	-2.093	-6.760	42.591	1.00	10.67
1338	N	GLY	A	107	-4.038	-7.137	41.536	1.00	11.50
1340	CA	GLY	A	107	-4.789	-6.222	42.368	1.00	12.10
1343	C	GLY	A	107	-4.904	-6.709	43.799	1.00	12.51
1344	O	GLY	A	107	-4.855	-5.913	44.743	1.00	12.78
1345	N	LYS	A	108	-5.083	-8.007	43.991	1.00	12.80
1347	CA	LYS	A	108	-5.153	-8.532	45.343	1.00	13.03
1349	CB	LYS	A	108	-5.596	-9.987	45.350	1.00	13.47
1352	CG	LYS	A	108	-5.960	-10.484	46.728	1.00	15.78
1355	CD	LYS	A	108	-6.618	-11.834	46.677	1.00	19.13
1358	CE	LYS	A	108	-6.632	-12.475	48.046	1.00	21.25
1361	NZ	LYS	A	108	-7.594	-13.604	48.096	1.00	23.85
1365	C	LYS	A	108	-3.814	-8.374	46.065	1.00	12.69
1366	O	LYS	A	108	-3.776	-8.068	47.262	1.00	13.21
1367	N	LEU	A	109	-2.726	-8.602	45.342	1.00	12.65
1369	CA	LEU	A	109	-1.393	-8.472	45.909	1.00	12.45
1371	CB	LEU	A	109	-0.340	-8.905	44.884	1.00	12.67
1374	CG	LEU	A	109	1.111	-8.728	45.334	1.00	13.11

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
1376	CD1	LEU	A	109	2.042	-9.118	44.188	1.00	14.19
1380	CD2	LEU	A	109	1.413	-9.539	46.591	1.00	13.65
1384	C	LEU	A	109	-1.127	-7.033	46.358	1.00	12.52
1385	O	LEU	A	109	-0.657	-6.800	47.471	1.00	12.92
1386	N	MET	A	110	-1.460	-6.065	45.500	1.00	12.89
1388	CA	MET	A	110	-1.206	-4.661	45.805	1.00	12.79
1390	CB	MET	A	110	-1.080	-3.840	44.513	1.00	12.79
1393	CG	MET	A	110	0.142	-4.178	43.690	1.00	11.94
1396	SD	MET	A	110	0.422	-3.011	42.350	1.00	12.63
1397	CE	MET	A	110	-0.927	-3.461	41.269	1.00	13.51
1401	C	MET	A	110	-2.277	-4.042	46.718	1.00	13.49
1402	O	MET	A	110	-2.071	-2.963	47.271	1.00	14.30
1403	N	GLY	A	111	-3.409	-4.720	46.881	1.00	13.28
1405	CA	GLY	A	111	-4.519	-4.191	47.663	1.00	13.54
1408	C	GLY	A	111	-5.317	-3.114	46.948	1.00	13.50
1409	O	GLY	A	111	-5.878	-2.227	47.586	1.00	14.56
1410	N	GLY	A	112	-5.361	-3.203	45.623	1.00	13.00
1412	CA	GLY	A	112	-6.103	-2.282	44.782	1.00	12.55
1415	C	GLY	A	112	-5.346	-2.001	43.489	1.00	12.44
1416	O	GLY	A	112	-4.335	-2.641	43.189	1.00	12.46
1417	N	LEU	A	113	-5.836	-1.022	42.737	1.00	11.74
1419	CA	LEU	A	113	-5.280	-0.680	41.429	1.00	11.64
1421	CB	LEU	A	113	-5.802	-1.629	40.351	1.00	11.77
1424	CG	LEU	A	113	-5.151	-1.465	38.971	1.00	12.59
1426	CD1	LEU	A	113	-3.678	-1.873	38.978	1.00	13.81
1430	CD2	LEU	A	113	-5.919	-2.252	37.916	1.00	14.21
1434	C	LEU	A	113	-5.660	0.745	41.072	1.00	11.50
1435	O	LEU	A	113	-6.850	1.092	41.061	1.00	11.30
1436	N	ASP	A	114	-4.644	1.554	40.778	1.00	11.48
1438	CA	ASP	A	114	-4.784	2.953	40.378	1.00	11.86
1440	CB	ASP	A	114	-3.778	3.817	41.139	1.00	11.83
1443	CG	ASP	A	114	-4.011	3.807	42.635	1.00	13.40
1444	OD1	ASP	A	114	-5.098	4.235	43.099	1.00	16.22
1445	OD2	ASP	A	114	-3.152	3.390	43.427	1.00	14.98
1446	C	ASP	A	114	-4.579	3.186	38.890	1.00	11.53
1447	O	ASP	A	114	-5.151	4.109	38.336	1.00	11.55
1448	N	MET	A	115	-3.743	2.374	38.239	1.00	11.65
1450	CA	MET	A	115	-3.446	2.581	36.821	1.00	12.03
1452	CB	MET	A	115	-2.270	3.550	36.646	1.00	12.51
1455	CG	MET	A	115	-1.948	3.910	35.194	1.00	13.35
1458	SD	MET	A	115	-0.643	5.145	35.023	1.00	17.9
1459	CE	MET	A	115	-1.525	6.634	35.502	1.00	18.97
1463	C	MET	A	115	-3.151	1.254	36.134	1.00	11.70
1464	O	MET	A	115	-2.366	0.441	36.633	1.00	12.00
1465	N	LEU	A	116	-3.780	1.061	34.981	1.00	11.39
1467	CA	LEU	A	116	-3.604	-0.119	34.157	1.00	11.20
1469	CB	LEU	A	116	-4.957	-0.748	33.859	1.00	11.28
1472	CG	LEU	A	116	-4.973	-1.946	32.922	1.00	11.66
1474	CD1	LEU	A	116	-4.340	-3.129	33.611	1.00	13.53

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
1478	CD2	LEU	A	116	-6.398	-2.256	32.505	1.00	12.30
1482	C	LEU	A	116	-2.944	0.329	32.861	1.00	11.25
1483	O	LEU	A	116	-3.557	1.040	32.070	1.00	11.10
1484	N	ILE	A	117	-1.690	-0.049	32.659	1.00	10.76
1486	CA	ILE	A	117	-0.968	0.336	31.445	1.00	11.16
1488	CB	ILE	A	117	0.443	0.864	31.754	1.00	11.32
1490	CG1	ILE	A	117	0.365	2.048	32.718	1.00	12.14
1493	CD1	ILE	A	117	1.718	2.649	33.085	1.00	13.08
1497	CG2	ILE	A	117	1.163	1.261	30.448	1.00	10.59
1501	C	ILE	A	117	-0.907	-0.879	30.539	1.00	10.80
1502	O	ILE	A	117	-0.235	-1.864	30.846	1.00	10.59
1503	N	LEU	A	118	-1.609	-0.784	29.417	1.00	10.45
1505	CA	LEU	A	118	-1.732	-1.854	28.434	1.00	10.13
1507	CB	LEU	A	118	-3.190	-1.930	27.966	1.00	10.43
1510	CG	LEU	A	118	-4.186	-2.138	29.110	1.00	10.25
1512	CD1	LEU	A	118	-5.625	-2.049	28.624	1.00	11.52
1516	CD2	LEU	A	118	-3.927	-3.471	29.815	1.00	11.22
1520	C	LEU	A	118	-0.797	-1.568	27.268	1.00	10.22
1521	O	LEU	A	118	-1.015	-0.627	26.509	1.00	10.36
1522	N	ASN	A	119	0.251	-2.377	27.144	1.00	9.88
1524	CA	ASN	A	119	1.373	-2.063	26.285	1.00	9.94
1526	CB	ASN	A	119	2.490	-1.486	27.186	1.00	9.71
1529	CG	ASN	A	119	3.851	-1.440	26.525	1.00	10.86
1530	OD1	ASN	A	119	4.697	-2.319	26.739	1.00	13.48
1531	ND2	ASN	A	119	4.082	-0.410	25.750	1.00	7.73
1534	C	ASN	A	119	1.844	-3.237	25.425	1.00	9.70
1535	O	ASN	A	119	2.441	-3.008	24.379	1.00	9.57
1536	N	HIS	A	120	1.582	-4.477	25.836	1.00	9.31
1538	CA	HIS	A	120	2.054	-5.640	25.081	1.00	9.34
1540	CB	HIS	A	120	1.725	-6.947	25.840	1.00	9.57
1543	CG	HIS	A	120	0.262	-7.147	26.072	1.00	9.97
1544	ND1	HIS	A	120	-0.567	-7.799	25.184	1.00	13.43
1546	CE1	HIS	A	120	-1.793	-7.812	25.668	1.00	8.49
1548	NE2	HIS	A	120	-1.797	-7.183	26.823	1.00	12.74
1550	CD2	HIS	A	120	-0.527	-6.745	27.091	1.00	7.45
1552	C	HIS	A	120	1.493	-5.733	23.665	1.00	8.99
1553	O	HIS	A	120	0.395	-5.263	23.376	1.00	9.09
1554	N	ILE	A	121	2.270	-6.356	22.783	1.00	8.63
1556	CA	ILE	A	121	1.820	-6.755	21.457	1.00	9.34
1558	CB	ILE	A	121	2.261	-5.744	20.363	1.00	9.34
1560	CG1	ILE	A	121	3.767	-5.475	20.427	1.00	10.84
1563	CD1	ILE	A	121	4.297	-4.741	19.213	1.00	12.35
1567	CG2	ILE	A	121	1.466	-4.461	20.477	1.00	9.17
1571	C	ILE	A	121	2.398	-8.118	21.134	1.00	9.37
1572	O	ILE	A	121	3.435	-8.527	21.693	1.00	10.57
1573	N	THR	A	122	1.754	-8.821	20.215	1.00	9.61
1575	CA	THR	A	122	2.313	-10.050	19.670	1.00	10.09
1577	CB	THR	A	122	1.200	-10.854	18.965	1.00	10.32
1579	OG1	THR	A	122	1.633	-12.200	18.744	1.00	10.54

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
1581	CG2	THR	A	122	0.878	-10.304	17.564	1.00	11.01
1585	C	THR	A	122	3.471	-9.689	18.719	1.00	11.46
1586	O	THR	A	122	3.517	-8.593	18.153	1.00	11.55
1587	N	ASN	A	123	4.415	-10.604	18.560	1.00	12.38
1589	CA	ASN	A	123	5.573	-10.352	17.721	1.00	14.10
1591	CB	ASN	A	123	6.510	-11.580	17.710	1.00	14.39
1594	CG	ASN	A	123	7.260	-11.784	19.026	1.00	16.38
1595	OD1	ASN	A	123	7.229	-10.951	19.942	1.00	18.79
1596	ND2	ASN	A	123	7.963	-12.916	19.119	1.00	20.92
1599	C	ASN	A	123	5.108	-10.017	16.295	1.00	15.12
1600	O	ASN	A	123	4.309	-10.743	15.696	1.00	14.58
1601	N	THR	A	124	5.568	-8.874	15.791	1.00	16.97
1603	CA	THR	A	124	5.209	-8.388	14.458	1.00	18.57
1605	CB	BTHR	A	124	4.234	-7.233	14.498	0.35	18.86
1606	CB	ATHR	A	124	4.159	-7.217	14.567	0.65	19.42
1609	OG1BTHR	A	124	4.870	-6.055	15.006	0.35	18.93	
1610	OG1ATHR	A	124	4.240	-6.326	13.445	0.65	19.80	
1613	CG2BTHR	A	124	3.176	-7.493	15.473	0.35	17.53	
1614	CG2ATHR	A	124	4.413	-6.269	15.740	0.65	18.06	
1621	C	THR	A	124	6.461	-7.944	13.728	1.00	20.02
1622	O	THR	A	124	7.250	-7.176	14.274	1.00	21.64
1623	N	SER	A	125	6.621	-8.423	12.509	1.00	20.65
1625	CA	SER	A	125	7.668	-7.921	11.617	1.00	21.51
1627	CB	SER	A	125	8.614	-9.046	11.217	1.00	21.79
1630	OG	SER	A	125	7.940	-10.023	10.464	1.00	25.57
1632	C	SER	A	125	7.052	-7.278	10.376	1.00	20.50
1633	O	SER	A	125	5.899	-7.530	10.027	1.00	20.85
1634	N	LEU	A	126	7.836	-6.435	9.716	1.00	19.49
1636	CA	LEU	A	126	7.371	-5.755	8.521	1.00	18.41
1638	CB	LEU	A	126	8.286	-4.575	8.220	1.00	18.30
1641	CG	LEU	A	126	8.235	-3.516	9.306	1.00	18.14
1643	CD1	LEU	A	126	9.363	-2.543	9.152	1.00	17.70
1647	CD2	LEU	A	126	6.892	-2.814	9.235	1.00	17.14
1651	C	LEU	A	126	7.367	-6.693	7.322	1.00	17.29
1652	O	LEU	A	126	8.410	-7.166	6.914	1.00	17.61
1653	N	ASN	A	127	6.195	-6.945	6.753	1.00	16.29
1655	CA	ASN	A	127	6.081	-7.737	5.532	1.00	16.45
1657	CB	ASN	A	127	6.286	-9.230	5.831	1.00	17.25
1660	CG	ASN	A	127	7.737	-9.691	5.641	1.00	20.22
1661	OD1	ASN	A	127	8.280	-10.409	6.483	1.00	25.21
1662	ND2	ASN	A	127	8.361	-9.279	4.545	1.00	23.68
1665	C	ASN	A	127	4.722	-7.538	4.872	1.00	15.39
1666	O	ASN	A	127	3.754	-7.186	5.547	1.00	14.23
1667	N	LEU	A	128	4.665	-7.732	3.558	1.00	14.25
1669	CA	LEU	A	128	3.399	-7.753	2.833	1.00	14.12
1671	CB	LEU	A	128	3.610	-8.129	1.371	1.00	14.18
1674	CG	LEU	A	128	4.298	-7.140	0.433	1.00	15.65
1676	CD1	LEU	A	128	4.803	-7.900	-0.784	1.00	17.00
1680	CD2	LEU	A	128	3.373	-6.025	0.013	1.00	16.03

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
1684	C	LEU	A	128	2.500	-8.803	3.456	1.00	14.04
1685	O	LEU	A	128	2.964	-9.867	3.849	1.00	14.34
1686	N	PHE	A	129	1.209	-8.509	3.539	1.00	13.84
1688	CA	PHE	A	129	0.243	-9.529	3.904	1.00	13.46
1690	CB	PHE	A	129	-1.152	-8.913	3.997	1.00	12.86
1693	CG	PHE	A	129	-2.220	-9.909	4.301	1.00	11.79
1694	CD1	PHE	A	129	-2.281	-10.515	5.545	1.00	12.71
1696	CE1	PHE	A	129	-3.258	-11.469	5.818	1.00	11.64
1698	CZ	PHE	A	129	-4.177	-11.791	4.857	1.00	12.44
1700	CE2	PHE	A	129	-4.126	-11.192	3.614	1.00	12.68
1702	CD2	PHE	A	129	-3.144	-10.251	3.338	1.00	12.21
1704	C	PHE	A	129	0.308	-10.645	2.857	1.00	14.16
1705	O	PHE	A	129	0.375	-10.386	1.659	1.00	14.99
1706	N	HIS	A	130	0.347	-11.892	3.313	1.00	14.55
1708	CA	HIS	A	130	0.555	-13.042	2.431	1.00	14.96
1710	CB	HIS	A	130	2.043	-13.456	2.416	1.00	15.55
1713	CG	HIS	A	130	2.616	-13.749	3.766	1.00	17.64
1714	ND1	HIS	A	130	2.910	-12.765	4.686	1.00	19.86
1716	CE1	HIS	A	130	3.398	-13.319	5.783	1.00	21.52
1718	NE2	HIS	A	130	3.421	-14.628	5.611	1.00	21.53
1720	CD2	HIS	A	130	2.945	-14.923	4.356	1.00	19.41
1722	C	HIS	A	130	-0.361	-14.210	2.815	1.00	14.69
1723	O	HIS	A	130	0.089	-15.345	2.967	1.00	15.10
1724	N	ASP	A	131	-1.656	-13.904	2.950	1.00	13.78
1726	CA	ASP	A	131	-2.715	-14.885	3.234	1.00	13.69
1728	CB	ASP	A	131	-2.770	-15.988	2.172	1.00	13.91
1731	CG	ASP	A	131	-3.050	-15.457	0.777	1.00	16.42
1732	OD1	ASP	A	131	-3.608	-14.346	0.647	1.00	17.50
1733	OD2	ASP	A	131	-2.746	-16.101	-0.255	1.00	20.24
1734	C	ASP	A	131	-2.598	-15.501	4.621	1.00	13.16
1735	O	ASP	A	131	-3.233	-16.526	4.915	1.00	13.46
1736	N	ASP	A	132	-1.803	-14.856	5.468	1.00	12.72
1738	CA	ASP	A	132	-1.529	-15.356	6.809	1.00	12.58
1740	CB	ASP	A	132	-0.125	-14.955	7.315	1.00	13.30
1743	CG	ASP	A	132	0.222	-13.480	7.089	1.00	14.42
1744	OD1	ASP	A	132	-0.096	-12.916	6.015	1.00	15.68
1745	OD2	ASP	A	132	0.888	-12.821	7.928	1.00	17.43
1746	C	ASP	A	132	-2.642	-14.911	7.753	1.00	12.19
1747	O	ASP	A	132	-2.423	-14.097	8.643	1.00	12.09
1748	N	ILE	A	133	-3.832	-15.481	7.548	1.00	12.08
1750	CA	ILE	A	133	-4.990	-15.203	8.392	1.00	12.44
1752	CB	ILE	A	133	-6.229	-16.000	7.916	1.00	12.91
1754	CG1	ILE	A	133	-6.642	-15.566	6.508	1.00	14.29
1757	CD1	ILE	A	133	-7.344	-16.624	5.762	1.00	17.50
1761	CG2	ILE	A	133	-7.410	-15.826	8.896	1.00	13.56
1765	C	ILE	A	133	-4.678	-15.507	9.850	1.00	12.67
1766	O	ILE	A	133	-5.167	-14.819	10.725	1.00	12.42
1767	N	HIS	A	134	-3.847	-16.521	10.116	1.00	12.82
1769	CA	HIS	A	134	-3.482	-16.869	11.496	1.00	12.94

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
1771	CB	HIS	A	134	-2.568	-18.134	11.568	1.00	13.10
1774	CG	HIS	A	134	-1.196	-17.966	10.970	1.00	13.12
1775	ND1	HIS	A	134	-0.148	-17.371	11.643	1.00	15.93
1777	CE1	HIS	A	134	0.922	-17.355	10.867	1.00	16.69
1779	NE2	HIS	A	134	0.617	-17.945	9.724	1.00	16.50
1781	CD2	HIS	A	134	-0.699	-18.345	9.766	1.00	15.53
1783	C	HIS	A	134	-2.853	-15.694	12.229	1.00	12.68
1784	O	HIS	A	134	-3.078	-15.492	13.420	1.00	12.80
1785	N	HIS	A	135	-2.060	-14.908	11.513	1.00	12.08
1787	CA	HIS	A	135	-1.415	-13.753	12.103	1.00	11.63
1789	CB	HIS	A	135	-0.262	-13.260	11.242	1.00	11.67
1792	CG	HIS	A	135	0.395	-12.023	11.763	1.00	14.39
1793	ND1	HIS	A	135	1.177	-12.007	12.902	1.00	16.83
1795	CE1	HIS	A	135	1.639	-10.784	13.091	1.00	17.41
1797	NE2	HIS	A	135	1.181	-10.007	12.130	1.00	17.28
1799	CD2	HIS	A	135	0.399	-10.757	11.287	1.00	16.70
1801	C	HIS	A	135	-2.389	-12.613	12.327	1.00	10.53
1802	O	HIS	A	135	-2.247	-11.899	13.293	1.00	10.95
1803	N	VAL	A	136	-3.366	-12.453	11.436	1.00	9.47
1805	CA	VAL	A	136	-4.389	-11.437	11.621	1.00	9.90
1807	CB	VAL	A	136	-5.338	-11.354	10.435	1.00	10.24
1809	CG1	VAL	A	136	-6.392	-10.270	10.664	1.00	11.29
1813	CG2	VAL	A	136	-4.542	-11.061	9.171	1.00	10.36
1817	C	VAL	A	136	-5.179	-11.764	12.876	1.00	9.81
1818	O	VAL	A	136	-5.443	-10.895	13.702	1.00	10.06
1819	N	ARG	A	137	-5.564	-13.026	13.022	1.00	10.01
1821	CA	ARG	A	137	-6.323	-13.448	14.193	1.00	10.98
1823	CB	ARG	A	137	-6.807	-14.889	14.047	1.00	11.57
1826	CG	ARG	A	137	-7.654	-15.347	15.227	1.00	15.06
1829	CD	BARG	A	137	-8.058	-16.806	15.159	0.35	16.94
1830	CD	AARG	A	137	-8.019	-16.814	15.183	0.65	19.73
1835	NE	BARG	A	137	-8.946	-17.072	14.028	0.35	18.67
1836	NE	AARG	A	137	-9.318	-17.062	14.571	0.65	24.03
1839	CZ	BARG	A	137	-10.264	-17.288	14.107	0.35	20.30
1840	CZ	AARG	A	137	-9.537	-17.327	13.281	0.65	27.17
1841	NH1BARG	A	137		-10.897	-17.284	15.276	0.35	20.86
1842	NH1AARG	A	137		-8.550	-17.355	12.386	0.65	26.90
1847	NH2BARG	A	137		-10.958	-17.522	12.999	0.35	22.20
1848	NH2AARG	A	137		-10.779	-17.547	12.874	0.65	29.51
1853	C	ARG	A	137	-5.513	-13.292	15.473	1.00	10.70
1854	O	ARG	A	137	-6.004	-12.764	16.468	1.00	10.51
1855	N	LYS	A	138	-4.257	-13.727	15.456	1.00	11.26
1857	CA	LYS	A	138	-3.411	-13.620	16.636	1.00	11.78
1859	CB	LYS	A	138	-2.072	-14.322	16.430	1.00	12.91
1862	CG	LYS	A	138	-1.176	-14.257	17.659	1.00	14.66
1865	CD	LYS	A	138	-0.040	-15.240	17.576	1.00	19.77
1868	CE	LYS	A	138	-0.517	-16.649	17.846	1.00	22.64
1871	NZ	LYS	A	138	0.610	-17.541	18.166	1.00	26.76
1875	C	LYS	A	138	-3.189	-12.164	17.026	1.00	11.49

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
1876	O	LYS	A	138	-3.230	-11.818	18.207	1.00	10.94
1877	N	SER	A	139	-2.997	-11.298	16.037	1.00	10.79
1879	CA	SER	A	139	-2.859	-9.871	16.305	1.00	10.57
1881	CB	SER	A	139	-2.588	-9.096	15.019	1.00	10.68
1884	OG	SER	A	139	-1.315	-9.439	14.525	1.00	11.59
1886	C	SER	A	139	-4.106	-9.314	16.979	1.00	10.43
1887	O	SER	A	139	-4.027	-8.544	17.940	1.00	9.90
1888	N	MET	A	140	-5.261	-9.708	16.467	1.00	10.90
1890	CA	MET	A	140	-6.512	-9.206	16.998	1.00	11.57
1892	CB	MET	A	140	-7.677	-9.587	16.082	1.00	12.12
1895	CG	MET	A	140	-7.762	-8.817	14.763	1.00	16.15
1898	SD	MET	A	140	-7.573	-6.992	14.809	1.00	21.70
1899	CE	MET	A	140	-8.504	-6.669	16.270	1.00	15.65
1903	C	MET	A	140	-6.709	-9.734	18.415	1.00	11.62
1904	O	MET	A	140	-7.138	-9.002	19.291	1.00	11.76
1905	N	GLU	A	141	-6.332	-10.978	18.679	1.00	10.59
1907	CA	GLU	A	141	-6.524	-11.531	20.034	1.00	11.31
1909	CB	GLU	A	141	-6.344	-13.050	20.027	1.00	12.33
1912	CG	GLU	A	141	-7.429	-13.796	19.269	1.00	15.26
1915	CD	GLU	A	141	-8.648	-14.108	20.113	1.00	20.89
1916	OE1	GLU	A	141	-9.742	-14.249	19.529	1.00	23.63
1917	OE2	GLU	A	141	-8.536	-14.203	21.357	1.00	23.33
1918	C	GLU	A	141	-5.579	-10.902	21.069	1.00	11.00
1919	O	GLU	A	141	-5.991	-10.503	22.154	1.00	11.40
1920	N	VAL	A	142	-4.297	-10.835	20.740	1.00	10.88
1922	CA	VAL	A	142	-3.290	-10.372	21.678	1.00	10.28
1924	CB	VAL	A	142	-1.885	-10.889	21.288	1.00	10.65
1926	CG1	VAL	A	142	-0.793	-10.288	22.187	1.00	10.71
1930	CG2	VAL	A	142	-1.879	-12.406	21.336	1.00	10.42
1934	C	VAL	A	142	-3.289	-8.850	21.787	1.00	10.10
1935	O	VAL	A	142	-3.265	-8.298	22.885	1.00	10.60
1936	N	ASN	A	143	-3.301	-8.170	20.652	1.00	9.47
1938	CA	ASN	A	143	-3.140	-6.725	20.660	1.00	9.48
1940	CB	ASN	A	143	-2.684	-6.219	19.290	1.00	9.32
1943	CG	ASN	A	143	-1.345	-6.783	18.841	1.00	10.46
1944	OD1	ASN	A	143	-0.684	-7.552	19.545	1.00	9.61
1945	ND2	ASN	A	143	-0.938	-6.389	17.633	1.00	10.58
1948	C	ASN	A	143	-4.408	-5.961	21.021	1.00	9.84
1949	O	ASN	A	143	-4.328	-4.795	21.388	1.00	10.52
1950	N	PHE	A	144	-5.567	-6.588	20.829	1.00	9.68
1952	CA	PHE	A	144	-6.865	-5.922	20.997	1.00	9.57
1954	CB	PHE	A	144	-7.627	-5.760	19.669	1.00	9.80
1957	CG	PHE	A	144	-9.049	-5.350	19.870	1.00	10.47
1958	CD1	PHE	A	144	-9.336	-4.092	20.350	1.00	11.74
1960	CE1	PHE	A	144	-10.640	-3.717	20.609	1.00	11.53
1962	CZ	PHE	A	144	-11.677	-4.612	20.401	1.00	10.73
1964	CE2	PHE	A	144	-11.409	-5.864	19.930	1.00	11.08
1966	CD2	PHE	A	144	-10.081	-6.244	19.682	1.00	10.03
1968	C	PHE	A	144	-7.732	-6.642	22.033	1.00	9.49

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
1969	O	PHE	A	144	-8.063	-6.063	23.067	1.00	9.71
1970	N	LEU	A	145	-8.123	-7.889	21.782	1.00	9.31
1972	CA	LEU	A	145	-9.106	-8.515	22.666	1.00	9.76
1974	CB	BLEU	A	145	-9.561	-9.878	22.139	0.35	9.81
1975	CB	ALEU	A	145	-9.553	-9.871	22.125	0.65	9.88
1980	CG	BLEU	A	145	-10.389	-9.860	20.855	0.35	10.79
1981	CG	ALEU	A	145	-10.759	-10.487	22.823	0.65	11.38
1984	CD1	BLEU	A	145	-10.573	-11.282	20.349	0.35	11.81
1985	CD1	ALEU	A	145	-11.991	-9.628	22.657	0.65	12.52
1992	CD2	BLEU	A	145	-11.742	-9.191	21.065	0.35	11.10
1993	CD2	ALEU	A	145	-10.987	-11.869	22.264	0.65	11.08
2000	C	LEU	A	145	-8.576	-8.648	24.082	1.00	9.40
2001	O	LEU	A	145	-9.307	-8.425	25.025	1.00	9.84
2002	N	SER	A	146	-7.295	-8.978	24.256	1.00	9.35
2004	CA	SER	A	146	-6.752	-9.101	25.604	1.00	9.51
2006	CB	SER	A	146	-5.335	-9.691	25.572	1.00	9.94
2009	OG	SER	A	146	-4.396	-8.717	25.179	1.00	10.50
2011	C	SER	A	146	-6.814	-7.766	26.366	1.00	9.75
2012	O	SER	A	146	-6.995	-7.743	27.581	1.00	9.24
2013	N	TYR	A	147	-6.692	-6.651	25.652	1.00	9.39
2015	CA	TYR	A	147	-6.786	-5.338	26.285	1.00	9.36
2017	CB	TYR	A	147	-6.460	-4.203	25.309	1.00	9.59
2020	CG	TYR	A	147	-4.993	-3.950	25.019	1.00	9.05
2021	CD1	TYR	A	147	-4.069	-4.994	24.912	1.00	9.72
2023	CE1	TYR	A	147	-2.724	-4.742	24.602	1.00	9.40
2025	CZ	TYR	A	147	-2.296	-3.434	24.439	1.00	9.98
2026	OH	TYR	A	147	-0.974	-3.132	24.148	1.00	10.82
2028	CE2	TYR	A	147	-3.205	-2.395	24.522	1.00	9.58
2030	CD2	TYR	A	147	-4.535	-2.654	24.820	1.00	9.53
2032	C	TYR	A	147	-8.192	-5.123	26.859	1.00	9.43
2033	O	TYR	A	147	-8.350	-4.530	27.928	1.00	10.12
2034	N	VAL	A	148	-9.202	-5.595	26.138	1.00	9.73
2036	CA	VAL	A	148	-10.592	-5.487	26.576	1.00	9.95
2038	CB	VAL	A	148	-11.564	-5.868	25.456	1.00	10.11
2040	CG1	VAL	A	148	-11.354	-4.975	24.232	1.00	10.02
2044	CG2	VAL	A	148	-12.994	-5.761	25.933	1.00	10.49
2048	C	VAL	A	148	-10.824	-6.375	27.807	1.00	9.78
2049	O	VAL	A	148	-11.442	-5.950	28.788	1.00	9.93
2050	N	VAL	A	149	-10.312	-7.601	27.768	1.00	9.80
2052	CA	VAL	A	149	-10.434	-8.526	28.904	1.00	10.03
2054	CB	VAL	A	149	-9.860	-9.924	28.540	1.00	10.01
2056	CG1	VAL	A	149	-9.764	-10.828	29.767	1.00	9.96
2060	CG2	VAL	A	149	-10.705	-10.562	27.460	1.00	10.49
2064	C	VAL	A	149	-9.759	-7.968	30.156	1.00	10.03
2065	O	VAL	A	149	-10.320	-7.994	31.253	1.00	10.05
2066	N	LEU	A	150	-8.562	-7.425	29.984	1.00	10.31
2068	CA	LEU	A	150	-7.843	-6.821	31.095	1.00	10.36
2070	CB	LEU	A	150	-6.463	-6.365	30.651	1.00	10.73
2073	CG	LEU	A	150	-5.505	-7.498	30.293	1.00	10.27



## FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
2075	CD1	LEU	A	150	-4.352	-6.974	29.438	1.00	9.37
2079	CD2	LEU	A	150	-4.964	-8.221	31.529	1.00	10.66
2083	C	LEU	A	150	-8.615	-5.643	31.692	1.00	10.37
2084	O	LEU	A	150	-8.681	-5.488	32.911	1.00	10.38
2085	N	THR	A	151	-9.218	-4.844	30.823	1.00	10.48
2087	CA	THR	A	151	-10.010	-3.698	31.241	1.00	10.79
2089	CB	THR	A	151	-10.419	-2.865	30.009	1.00	10.86
2091	OG1	THR	A	151	-9.260	-2.244	29.452	1.00	12.66
2093	CG2	THR	A	151	-11.333	-1.705	30.392	1.00	12.19
2097	C	THR	A	151	-11.227	-4.117	32.052	1.00	10.65
2098	O	THR	A	151	-11.502	-3.535	33.100	1.00	10.75
2099	N	VAL	A	152	-11.960	-5.113	31.565	1.00	10.74
2101	CA	VAL	A	152	-13.139	-5.622	32.263	1.00	10.86
2103	CB	VAL	A	152	-13.815	-6.755	31.450	1.00	11.39
2105	CG1	VAL	A	152	-14.831	-7.510	32.269	1.00	12.64
2109	CG2	VAL	A	152	-14.462	-6.196	30.145	1.00	11.40
2113	C	VAL	A	152	-12.725	-6.121	33.645	1.00	11.38
2114	O	VAL	A	152	-13.421	-5.887	34.636	1.00	11.46
2115	N	ALA	A	153	-11.591	-6.804	33.723	1.00	10.80
2117	CA	ALA	A	153	-11.148	-7.358	35.005	1.00	11.47
2119	CB	ALA	A	153	-10.009	-8.341	34.794	1.00	11.43
2123	C	ALA	A	153	-10.717	-6.267	35.975	1.00	11.90
2124	O	ALA	A	153	-10.873	-6.410	37.187	1.00	12.37
2125	N	ALA	A	154	-10.178	-5.174	35.441	1.00	11.38
2127	CA	ALA	A	154	-9.612	-4.110	36.260	1.00	11.55
2129	CB	ALA	A	154	-8.488	-3.419	35.507	1.00	11.90
2133	C	ALA	A	154	-10.630	-3.070	36.691	1.00	11.82
2134	O	ALA	A	154	-10.391	-2.341	37.648	1.00	11.16
2135	N	LEU	A	155	-11.750	-2.973	35.987	1.00	12.39
2137	CA	LEU	A	155	-12.607	-1.791	36.134	1.00	12.82
2139	CB	LEU	A	155	-13.740	-1.756	35.101	1.00	12.77
2142	CG	LEU	A	155	-14.514	-0.431	35.006	1.00	15.39
2144	CD1	LEU	A	155	-15.632	-0.564	33.976	1.00	17.15
2148	CD2	LEU	A	155	-13.602	0.739	34.655	1.00	17.18
2152	C	LEU	A	155	-13.173	-1.615	37.544	1.00	12.83
2153	O	LEU	A	155	-13.194	-0.492	38.021	1.00	12.68
2154	N	PRO	A	156	-13.640	-2.675	38.211	1.00	12.68
2155	CA	PRO	A	156	-14.124	-2.510	39.594	1.00	12.84
2157	CB	PRO	A	156	-14.466	-3.937	40.017	1.00	13.08
2160	CG	PRO	A	156	-14.799	-4.628	38.743	1.00	13.53
2163	CD	PRO	A	156	-13.830	-4.055	37.740	1.00	12.49
2166	C	PRO	A	156	-13.091	-1.843	40.525	1.00	12.92
2167	O	PRO	A	156	-13.441	-0.907	41.251	1.00	12.97
2168	N	MET	A	157	-11.838	-2.283	40.465	1.00	12.85
2170	CA	MET	A	157	-10.765	-1.671	41.246	1.00	12.60
2172	CB	MET	A	157	-9.483	-2.510	41.171	1.00	12.58
2175	CG	MET	A	157	-9.530	-3.778	41.991	1.00	12.57
2178	SD	MET	A	157	-7.980	-4.666	41.958	1.00	14.98
2179	CE	MET	A	157	-7.953	-5.260	40.271	1.00	15.15

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
2183	C	MET	A	157	-10.482	-0.232	40.803	1.00	12.35
2184	O	MET	A	157	-10.263	0.640	41.640	1.00	12.09
2185	N	LEU	A	158	-10.508	0.023	39.496	1.00	12.12
2187	CA	LEU	A	158	-10.266	1.368	38.983	1.00	12.51
2189	CB	LEU	A	158	-10.066	1.346	37.469	1.00	12.39
2192	CG	LEU	A	158	-8.788	0.628	37.016	1.00	12.88
2194	CD1	LEU	A	158	-8.797	0.481	35.503	1.00	13.53
2198	CD2	LEU	A	158	-7.556	1.368	37.469	1.00	13.52
2202	C	LEU	A	158	-11.394	2.329	39.371	1.00	12.39
2203	O	LEU	A	158	-11.148	3.499	39.609	1.00	12.45
2204	N	LYS	A	159	-12.620	1.824	39.449	1.00	13.18
2206	CA	LYS	A	159	-13.756	2.635	39.889	1.00	14.15
2208	CB	LYS	A	159	-15.069	1.894	39.640	1.00	14.39
2211	CG	LYS	A	159	-15.513	1.911	38.187	1.00	15.23
2214	CD	LYS	A	159	-16.683	0.953	37.933	1.00	17.07
2217	CE	LYS	A	159	-17.364	1.231	36.602	1.00	19.52
2220	NZ	LYS	A	159	-18.301	0.142	36.175	1.00	20.70
2224	C	LYS	A	159	-13.605	2.998	41.369	1.00	15.38
2225	O	LYS	A	159	-13.919	4.117	41.781	1.00	15.86
2226	N	GLN	A	160	-13.112	2.050	42.158	1.00	15.84
2228	CA	GLN	A	160	-12.839	2.278	43.577	1.00	16.84
2230	CB	GLN	A	160	-12.348	0.982	44.224	1.00	17.43
2233	CG	GLN	A	160	-12.344	0.967	45.729	1.00	21.62
2236	CD	GLN	A	160	-13.631	0.403	46.284	1.00	26.11
2237	OE1	GLN	A	160	-14.560	1.154	46.580	1.00	29.04
2238	NE2	GLN	A	160	-13.701	-0.928	46.402	1.00	29.33
2241	C	GLN	A	160	-11.808	3.391	43.808	1.00	16.54
2242	O	GLN	A	160	-11.930	4.165	44.760	1.00	17.68
2243	N	SER	A	161	-10.807	3.475	42.938	1.00	15.57
2245	CA	SER	A	161	-9.701	4.422	43.081	1.00	14.86
2247	CB	SER	A	161	-8.376	3.721	42.759	1.00	15.18
2250	OG	SER	A	161	-8.316	3.375	41.386	1.00	14.71
2252	C	SER	A	161	-9.814	5.667	42.191	1.00	14.85
2253	O	SER	A	161	-8.935	6.527	42.227	1.00	14.62
2254	N	ASN	A	162	-10.884	5.772	41.411	1.00	14.79
2256	CA	ASN	A	162	-10.988	6.811	40.378	1.00	15.06
2258	CB	ASN	A	162	-11.199	8.198	40.992	1.00	15.40
2261	CG	ASN	A	162	-12.416	8.254	41.888	1.00	17.57
2262	OD1	ASN	A	162	-13.511	7.885	41.480	1.00	19.52
2263	ND2	ASN	A	162	-12.224	8.699	43.126	1.00	21.95
2266	C	ASN	A	162	-9.734	6.811	39.516	1.00	14.16
2267	O	ASN	A	162	-9.111	7.851	39.292	1.00	14.61
2268	N	GLY	A	163	-9.370	5.615	39.056	1.00	13.36
2270	CA	GLY	A	163	-8.097	5.359	38.410	1.00	12.86
2273	C	GLY	A	163	-8.062	5.641	36.925	1.00	12.81
2274	O	GLY	A	163	-8.877	6.377	36.398	1.00	12.37
2275	N	SER	A	164	-7.097	5.028	36.247	1.00	12.80
2277	CA	SER	A	164	-6.765	5.379	34.876	1.00	13.04
2279	CB	SER	A	164	-5.600	6.363	34.868	1.00	13.40

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
2282	OG	SER	A	164	-5.888	7.538	35.611	1.00	15.44
2284	C	SER	A	164	-6.368	4.148	34.085	1.00	12.49
2285	O	SER	A	164	-5.697	3.260	34.614	1.00	13.06
2286	N	ILE	A	165	-6.787	4.120	32.825	1.00	12.11
2288	CA	ILE	A	165	-6.377	3.128	31.839	1.00	11.44
2290	CB	ILE	A	165	-7.613	2.488	31.157	1.00	11.74
2292	CG1	ILE	A	165	-8.518	1.821	32.197	1.00	13.03
2295	CD1	ILE	A	165	-9.872	1.441	31.667	1.00	13.40
2299	CG2	ILE	A	165	-7.182	1.502	30.075	1.00	12.06
2303	C	ILE	A	165	-5.515	3.829	30.796	1.00	11.39
2304	O	ILE	A	165	-5.897	4.877	30.272	1.00	11.10
2305	N	VAL	A	166	-4.347	3.264	30.514	1.00	11.09
2307	CA	VAL	A	166	-3.458	3.790	29.483	1.00	11.11
2309	CB	VAL	A	166	-2.079	4.175	30.062	1.00	11.42
2311	CG1	VAL	A	166	-1.124	4.655	28.965	1.00	12.56
2315	CG2	VAL	A	166	-2.246	5.226	31.161	1.00	13.43
2319	C	VAL	A	166	-3.308	2.708	28.434	1.00	11.10
2320	O	VAL	A	166	-2.929	1.580	28.749	1.00	11.97
2321	N	VAL	A	167	-3.628	3.060	27.195	1.00	10.73
2323	CA	VAL	A	167	-3.582	2.151	26.062	1.00	10.77
2325	CB	VAL	A	167	-4.935	2.123	25.327	1.00	10.86
2327	CG1	VAL	A	167	-4.875	1.225	24.097	1.00	11.39
2331	CG2	VAL	A	167	-6.045	1.673	26.282	1.00	11.58
2335	C	VAL	A	167	-2.489	2.636	25.119	1.00	10.62
2336	O	VAL	A	167	-2.558	3.743	24.596	1.00	10.55
2337	N	VAL	A	168	-1.475	1.810	24.900	1.00	10.22
2339	CA	VAL	A	168	-0.361	2.201	24.049	1.00	10.27
2341	CB	VAL	A	168	0.984	1.606	24.515	1.00	9.63
2343	CG1	VAL	A	168	2.117	2.099	23.622	1.00	10.86
2347	CG2	VAL	A	168	1.252	1.988	25.943	1.00	9.25
2351	C	VAL	A	168	-0.654	1.806	22.616	1.00	10.04
2352	O	VAL	A	168	-0.931	0.646	22.308	1.00	10.47
2353	N	SER	A	169	-0.617	2.810	21.750	1.00	10.28
2355	CA	SER	A	169	-0.841	2.641	20.318	1.00	9.68
2357	CB	SER	A	169	-2.273	3.092	19.970	1.00	9.85
2360	OG	SER	A	169	-2.623	2.745	18.638	1.00	10.29
2362	C	SER	A	169	0.244	3.361	19.514	1.00	10.36
2363	O	SER	A	169	1.365	3.545	20.001	1.00	11.28
2364	N	SER	A	170	-0.079	3.769	18.291	1.00	9.75
2366	CA	SER	A	170	0.897	3.796	17.215	1.00	9.23
2368	CB	SER	A	170	0.989	2.401	16.584	1.00	10.00
2371	OG	SER	A	170	1.023	1.394	17.582	1.00	11.18
2373	C	SER	A	170	0.457	4.753	16.141	1.00	9.33
2374	O	SER	A	170	-0.739	4.920	15.906	1.00	9.26
2375	N	LEU	A	171	1.415	5.317	15.415	1.00	8.94
2377	CA	LEU	A	171	1.076	6.055	14.202	1.00	9.38
2379	CB	LEU	A	171	2.324	6.525	13.456	1.00	9.67
2382	CG	LEU	A	171	3.122	7.641	14.131	1.00	10.64
2384	CD1	LEU	A	171	2.294	8.904	14.291	1.00	13.15

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
2388	CD2	LEU	A	171	4.354	7.912	13.294	1.00	10.42
2392	C	LEU	A	171	0.223	5.196	13.266	1.00	9.37
2393	O	LEU	A	171	-0.720	5.698	12.673	1.00	8.49
2394	N	ALA	A	172	0.531	3.898	13.180	1.00	9.28
2396	CA	ALA	A	172	-0.200	2.977	12.317	1.00	9.84
2398	CB	ALA	A	172	0.667	1.744	11.983	1.00	9.62
2402	C	ALA	A	172	-1.539	2.558	12.925	1.00	9.83
2403	O	ALA	A	172	-2.225	1.690	12.384	1.00	10.17
2404	N	GLY	A	173	-1.882	3.163	14.061	1.00	9.67
2406	CA	GLY	A	173	-3.196	3.089	14.665	1.00	9.91
2409	C	GLY	A	173	-4.021	4.354	14.431	1.00	9.85
2410	O	GLY	A	173	-5.139	4.451	14.949	1.00	10.98
2411	N	LYS	A	174	-3.481	5.306	13.658	1.00	9.32
2413	CA	LYS	A	174	-4.178	6.560	13.325	1.00	9.25
2415	CB	LYS	A	174	-3.560	7.745	14.062	1.00	9.54
2418	CG	LYS	A	174	-3.833	7.755	15.551	1.00	9.69
2421	CD	LYS	A	174	-5.304	8.057	15.845	1.00	10.41
2424	CE	LYS	A	174	-5.570	8.386	17.304	1.00	11.00
2427	NZ	LYS	A	174	-7.027	8.698	17.564	1.00	10.52
2431	C	LYS	A	174	-4.218	6.844	11.819	1.00	9.39
2432	O	LYS	A	174	-5.151	7.486	11.328	1.00	10.14
2433	N	VAL	A	175	-3.213	6.377	11.099	1.00	10.06
2435	CA	VAL	A	175	-3.185	6.449	9.651	1.00	10.50
2437	CB	VAL	A	175	-2.324	7.627	9.133	1.00	10.72
2439	CG1	VAL	A	175	-0.872	7.431	9.479	1.00	11.95
2443	CG2	VAL	A	175	-2.857	8.952	9.680	1.00	11.47
2447	C	VAL	A	175	-2.673	5.119	9.126	1.00	10.60
2448	O	VAL	A	175	-2.152	4.296	9.886	1.00	11.55
2449	N	ALA	A	176	-2.837	4.908	7.830	1.00	11.32
2451	CA	ALA	A	176	-2.532	3.628	7.218	1.00	11.97
2453	CB	ALA	A	176	-3.555	3.311	6.138	1.00	12.29
2457	C	ALA	A	176	-1.119	3.584	6.631	1.00	11.96
2458	O	ALA	A	176	-0.624	4.559	6.080	1.00	12.93
2459	N	TYR	A	177	-0.493	2.423	6.769	1.00	11.82
2461	CA	TYR	A	177	0.819	2.128	6.231	1.00	11.75
2463	CB	TYR	A	177	1.833	2.043	7.372	1.00	12.18
2466	CG	TYR	A	177	2.184	3.341	8.045	1.00	10.90
2467	CD1	TYR	A	177	1.415	3.836	9.081	1.00	11.58
2469	CE1	TYR	A	177	1.736	5.023	9.725	1.00	11.10
2471	CZ	TYR	A	177	2.858	5.713	9.360	1.00	12.21
2472	OH	TYR	A	177	3.150	6.879	10.028	1.00	11.86
2474	CE2	TYR	A	177	3.654	5.248	8.330	1.00	11.31
2476	CD2	TYR	A	177	3.309	4.055	7.677	1.00	11.35
2478	C	TYR	A	177	0.799	0.752	5.585	1.00	11.78
2479	O	TYR	A	177	0.170	-0.165	6.123	1.00	12.50
2480	N	PRO	A	178	1.579	0.537	4.535	1.00	11.47
2481	CA	PRO	A	178	1.759	-0.829	4.046	1.00	11.34
2483	CB	PRO	A	178	2.470	-0.625	2.721	1.00	11.47
2486	CG	PRO	A	178	3.283	0.594	2.963	1.00	11.38

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
2489	CD	PRO	A	178	2.441	1.495	3.812	1.00	11.15
2492	C	PRO	A	178	2.640	-1.592	5.027	1.00	11.07
2493	O	PRO	A	178	3.340	-0.979	5.830	1.00	11.92
2494	N	MET	A	179	2.612	-2.917	4.939	1.00	10.90
2496	CA	MET	A	179	3.525	-3.838	5.620	1.00	10.85
2498	CB	MET	A	179	5.002	-3.405	5.504	1.00	11.24
2501	CG	MET	A	179	5.431	-2.934	4.106	1.00	12.33
2504	SD	MET	A	179	4.958	-4.077	2.815	1.00	16.35
2505	CE	MET	A	179	5.406	-3.132	1.336	1.00	16.92
2509	C	MET	A	179	3.194	-4.123	7.082	1.00	10.20
2510	O	MET	A	179	3.893	-4.908	7.735	1.00	10.26
2511	N	VAL	A	180	2.133	-3.498	7.589	1.00	10.46
2513	CA	VAL	A	180	1.686	-3.690	8.958	1.00	10.18
2515	CB	VAL	A	180	2.099	-2.510	9.876	1.00	10.81
2517	CG1	VAL	A	180	3.601	-2.493	10.074	1.00	11.63
2521	CG2	VAL	A	180	1.624	-1.172	9.314	1.00	10.87
2525	C	VAL	A	180	0.170	-3.866	9.015	1.00	10.05
2526	O	VAL	A	180	-0.467	-3.440	9.976	1.00	10.08
2527	N	ALA	A	181	-0.405	-4.535	8.017	1.00	9.27
2529	CA	ALA	A	181	-1.882	-4.636	7.917	1.00	9.51
2531	CB	ALA	A	181	-2.275	-5.403	6.690	1.00	9.85
2535	C	ALA	A	181	-2.556	-5.226	9.160	1.00	9.14
2536	O	ALA	A	181	-3.494	-4.640	9.697	1.00	9.12
2537	N	ALA	A	182	-2.109	-6.396	9.596	1.00	9.20
2539	CA	ALA	A	182	-2.663	-7.049	10.769	1.00	9.32
2541	CB	ALA	A	182	-2.004	-8.400	10.945	1.00	9.17
2545	C	ALA	A	182	-2.498	-6.209	12.031	1.00	9.02
2546	O	ALA	A	182	-3.424	-6.082	12.843	1.00	9.75
2547	N	TYR	A	183	-1.315	-5.630	12.214	1.00	8.82
2549	CA	TYR	A	183	-1.044	-4.806	13.378	1.00	8.63
2551	CB	TYR	A	183	0.420	-4.406	13.328	1.00	8.65
2554	CG	TYR	A	183	0.886	-3.376	14.321	1.00	8.36
2555	CD1	TYR	A	183	1.344	-3.748	15.578	1.00	8.05
2557	CE1	TYR	A	183	1.825	-2.832	16.477	1.00	8.32
2559	CZ	TYR	A	183	1.842	-1.497	16.136	1.00	7.64
2560	OH	TYR	A	183	2.376	-0.557	16.978	1.00	9.96
2562	CE2	TYR	A	183	1.387	-1.095	14.891	1.00	8.43
2564	CD2	TYR	A	183	0.911	-2.026	14.000	1.00	8.34
2566	C	TYR	A	183	-1.923	-3.561	13.370	1.00	8.82
2567	O	TYR	A	183	-2.487	-3.184	14.378	1.00	9.23
2568	N	SER	A	184	-2.007	-2.907	12.221	1.00	9.00
2570	CA	SER	A	184	-2.782	-1.672	12.094	1.00	9.32
2572	CB	BSER	A	184	-2.661	-1.084	10.688	0.35	9.53
2573	CB	ASER	A	184	-2.593	-1.106	10.683	0.65	9.67
2578	OG	BSER	A	184	-1.412	-0.455	10.514	0.35	10.17
2579	OG	ASER	A	184	-3.287	0.105	10.502	0.65	10.17
2582	C	SER	A	184	-4.245	-1.938	12.404	1.00	9.29
2583	O	SER	A	184	-4.893	-1.165	13.124	1.00	9.06
2584	N	ALA	A	185	-4.761	-3.056	11.910	1.00	8.76

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
2586	CA	ALA	A	185	-6.148	-3.426	12.198	1.00	8.85
2588	CB	ALA	A	185	-6.494	-4.761	11.598	1.00	8.88
2592	C	ALA	A	185	-6.354	-3.454	13.707	1.00	8.75
2593	O	ALA	A	185	-7.371	-2.954	14.226	1.00	8.86
2594	N	SER	A	186	-5.415	-4.070	14.426	1.00	8.55
2596	CA	SER	A	186	-5.557	-4.211	15.869	1.00	8.54
2598	CB	SER	A	186	-4.570	-5.252	16.424	1.00	9.15
2601	OG	SER	A	186	-3.249	-4.756	16.482	1.00	9.38
2603	C	SER	A	186	-5.461	-2.879	16.609	1.00	8.52
2604	O	SER	A	186	-6.173	-2.648	17.583	1.00	8.63
2605	N	LYS	A	187	-4.580	-1.985	16.159	1.00	8.62
2607	CA	LYS	A	187	-4.427	-0.694	16.814	1.00	8.42
2609	CB	LYS	A	187	-3.070	-0.062	16.490	1.00	8.79
2612	CG	LYS	A	187	-1.852	-0.869	16.992	1.00	9.32
2615	CD	LYS	A	187	-1.827	-0.991	18.513	1.00	8.80
2618	CE	LYS	A	187	-0.421	-1.296	19.029	1.00	10.25
2621	NZ	LYS	A	187	-0.381	-1.481	20.519	1.00	8.76
2625	C	LYS	A	187	-5.576	0.263	16.470	1.00	8.49
2626	O	LYS	A	187	-6.017	1.012	17.336	1.00	8.32
2627	N	PHE	A	188	-6.056	0.246	15.230	1.00	8.45
2629	CA	PHE	A	188	-7.278	0.966	14.873	1.00	8.30
2631	CB	PHE	A	188	-7.648	0.779	13.402	1.00	8.39
2634	CG	PHE	A	188	-7.051	1.812	12.463	1.00	8.04
2635	CD1	PHE	A	188	-7.864	2.716	11.792	1.00	8.36
2637	CE1	PHE	A	188	-7.326	3.645	10.894	1.00	9.29
2639	CZ	PHE	A	188	-5.952	3.701	10.679	1.00	8.98
2641	CE2	PHE	A	188	-5.128	2.801	11.327	1.00	9.29
2643	CD2	PHE	A	188	-5.672	1.862	12.225	1.00	8.93
2645	C	PHE	A	188	-8.433	0.479	15.761	1.00	8.62
2646	O	PHE	A	188	-9.204	1.290	16.261	1.00	8.60
2647	N	ALA	A	189	-8.540	-0.828	15.964	1.00	8.26
2649	CA	ALA	A	189	-9.620	-1.377	16.807	1.00	8.33
2651	CB	ALA	A	189	-9.559	-2.888	16.848	1.00	8.27
2655	C	ALA	A	189	-9.547	-0.826	18.221	1.00	8.44
2656	O	ALA	A	189	-10.574	-0.525	18.826	1.00	9.04
2657	N	LEU	A	190	-8.339	-0.683	18.761	1.00	8.88
2659	CA	LEU	A	190	-8.194	-0.119	20.098	1.00	9.01
2661	CB	LEU	A	190	-6.741	-0.085	20.544	1.00	9.20
2664	CG	LEU	A	190	-6.083	-1.417	20.904	1.00	9.09
2666	CD1	LEU	A	190	-4.596	-1.193	21.064	1.00	10.39
2670	CD2	LEU	A	190	-6.645	-2.024	22.173	1.00	9.95
2674	C	LEU	A	190	-8.768	1.288	20.168	1.00	8.96
2675	O	LEU	A	190	-9.393	1.646	21.144	1.00	8.84
2676	N	ASP	A	191	-8.509	2.100	19.150	1.00	9.44
2678	CA	ASP	A	191	-9.001	3.469	19.116	1.00	9.93
2680	CB	ASP	A	191	-8.433	4.175	17.890	1.00	9.70
2683	CG	ASP	A	191	-8.724	5.656	17.848	1.00	10.93
2684	OD1	ASP	A	191	-9.300	6.226	18.803	1.00	10.92
2685	OD2	ASP	A	191	-8.353	6.323	16.869	1.00	10.94

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
2686	C	ASP	A	191	-10.526	3.465	19.097	1.00	9.95
2687	O	ASP	A	191	-11.170	4.129	19.909	1.00	10.49
2688	N	GLY	A	192	-11.118	2.682	18.199	1.00	9.32
2690	CA	GLY	A	192	-12.564	2.629	18.110	1.00	9.37
2693	C	GLY	A	192	-13.189	2.187	19.415	1.00	9.15
2694	O	GLY	A	192	-14.144	2.810	19.896	1.00	10.23
2695	N	PHE	A	193	-12.658	1.107	19.995	1.00	9.24
2697	CA	PHE	A	193	-13.226	0.556	21.238	1.00	9.38
2699	CB	PHE	A	193	-12.603	-0.793	21.619	1.00	9.61
2702	CG	PHE	A	193	-13.322	-1.467	22.751	1.00	10.09
2703	CD1	PHE	A	193	-12.887	-1.331	24.052	1.00	10.77
2705	CE1	PHE	A	193	-13.593	-1.930	25.097	1.00	12.22
2707	CZ	PHE	A	193	-14.725	-2.660	24.819	1.00	11.76
2709	CE2	PHE	A	193	-15.161	-2.807	23.536	1.00	12.81
2711	CD2	PHE	A	193	-14.473	-2.207	22.499	1.00	11.18
2713	C	PHE	A	193	-13.058	1.500	22.413	1.00	9.54
2714	O	PHE	A	193	-14.029	1.860	23.072	1.00	9.87
2715	N	PHE	A	194	-11.824	1.891	22.687	1.00	9.19
2717	CA	PHE	A	194	-11.552	2.684	23.880	1.00	9.61
2719	CB	PHE	A	194	-10.075	2.618	24.262	1.00	9.96
2722	CG	PHE	A	194	-9.719	1.322	24.943	1.00	10.17
2723	CD1	PHE	A	194	-9.227	0.244	24.226	1.00	10.38
2725	CE1	PHE	A	194	-8.938	-0.964	24.861	1.00	11.43
2727	CZ	PHE	A	194	-9.148	-1.106	26.225	1.00	12.52
2729	CE2	PHE	A	194	-9.640	-0.044	26.947	1.00	11.80
2731	CD2	PHE	A	194	-9.937	1.163	26.306	1.00	10.54
2733	C	PHE	A	194	-12.099	4.093	23.806	1.00	9.59
2734	O	PHE	A	194	-12.484	4.651	24.814	1.00	9.70
2735	N	SER	A	195	-12.141	4.663	22.612	1.00	10.39
2737	CA	SER	A	195	-12.743	5.980	22.427	1.00	10.54
2739	CB	SER	A	195	-12.388	6.553	21.058	1.00	10.93
2742	OG	SER	A	195	-10.998	6.759	20.940	1.00	10.86
2744	C	SER	A	195	-14.257	5.933	22.622	1.00	11.03
2745	O	SER	A	195	-14.850	6.887	23.107	1.00	10.66
2746	N	SER	A	196	-14.886	4.815	22.265	1.00	10.79
2748	CA	SER	A	196	-16.317	4.636	22.494	1.00	11.34
2750	CB	BSER	A	196	-16.833	3.434	21.714	0.35	11.27
2751	CB	ASER	A	196	-16.844	3.395	21.764	0.65	11.24
2756	OG	BSER	A	196	-16.762	3.705	20.325	0.35	11.84
2757	OG	ASER	A	196	-18.198	3.103	22.111	0.65	11.84
2760	C	SER	A	196	-16.608	4.490	23.976	1.00	11.43
2761	O	SER	A	196	-17.517	5.147	24.504	1.00	11.84
2762	N	ILE	A	197	-15.856	3.649	24.679	1.00	11.39
2764	CA	ILE	A	197	-16.154	3.482	26.100	1.00	12.56
2766	CB	ILE	A	197	-15.563	2.192	26.723	1.00	13.89
2768	CG1	ILE	A	197	-14.057	2.144	26.648	1.00	14.45
2771	CD1	ILE	A	197	-13.456	1.071	27.548	1.00	16.54
2775	CG2	ILE	A	197	-16.198	0.933	26.111	1.00	14.40
2779	C	ILE	A	197	-15.800	4.742	26.890	1.00	12.22

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
2780	O	ILE	A	197	-16.446	5.036	27.887	1.00	12.16
2781	N	ARG	A	198	-14.859	5.553	26.401	1.00	12.12
2783	CA	ARG	A	198	-14.606	6.844	27.039	1.00	12.80
2785	CB	ARG	A	198	-13.487	7.619	26.346	1.00	13.27
2788	CG	ARG	A	198	-13.020	8.826	27.144	1.00	14.48
2791	CD	ARG	A	198	-12.051	9.729	26.426	1.00	14.81
2794	NE	ARG	A	198	-10.717	9.141	26.267	1.00	13.09
2796	CZ	ARG	A	198	-10.156	8.816	25.103	1.00	13.72
2797	NH1	ARG	A	198	-10.827	8.929	23.964	1.00	13.58
2800	NH2	ARG	A	198	-8.921	8.330	25.070	1.00	14.23
2803	C	ARG	A	198	-15.879	7.689	27.048	1.00	12.92
2804	O	ARG	A	198	-16.217	8.286	28.066	1.00	13.72
2805	N	LYS	A	199	-16.574	7.721	25.919	1.00	12.71
2807	CA	LYS	A	199	-17.831	8.469	25.815	1.00	13.22
2809	CB	LYS	A	199	-18.274	8.557	24.354	1.00	13.79
2812	CG	LYS	A	199	-17.408	9.553	23.565	1.00	15.53
2815	CD	LYS	A	199	-17.547	9.396	22.078	1.00	17.33
2818	CE	LYS	A	199	-16.587	10.314	21.310	1.00	16.43
2821	NZ	LYS	A	199	-16.358	11.685	21.864	1.00	15.91
2825	C	LYS	A	199	-18.912	7.872	26.719	1.00	13.58
2826	O	LYS	A	199	-19.685	8.610	27.328	1.00	13.87
2827	N	GLU	A	200	-18.948	6.546	26.813	1.00	12.75
2829	CA	GLU	A	200	-19.884	5.871	27.708	1.00	13.49
2831	CB	GLU	A	200	-19.849	4.360	27.500	1.00	13.22
2834	CG	GLU	A	200	-20.362	3.940	26.141	1.00	14.14
2837	CD	GLU	A	200	-20.343	2.440	25.930	1.00	14.08
2838	OE1	GLU	A	200	-20.600	2.019	24.788	1.00	15.20
2839	OE2	GLU	A	200	-20.087	1.691	26.890	1.00	14.89
2840	C	GLU	A	200	-19.601	6.224	29.161	1.00	13.89
2841	O	GLU	A	200	-20.529	6.496	29.914	1.00	13.96
2842	N	TYR	A	201	-18.329	6.278	29.547	1.00	14.36
2844	CA	TYR	A	201	-17.983	6.609	30.934	1.00	15.15
2846	CB	TYR	A	201	-16.494	6.357	31.232	1.00	15.43
2849	CG	TYR	A	201	-16.083	4.893	31.212	1.00	15.96
2850	CD1	TYR	A	201	-17.019	3.875	31.009	1.00	17.82
2852	CE1	TYR	A	201	-16.646	2.539	30.991	1.00	19.88
2854	CZ	TYR	A	201	-15.327	2.195	31.150	1.00	20.30
2855	OH	TYR	A	201	-14.979	0.858	31.108	1.00	24.41
2857	CE2	TYR	A	201	-14.368	3.168	31.350	1.00	19.93
2859	CD2	TYR	A	201	-14.750	4.524	31.381	1.00	18.36
2861	C	TYR	A	201	-18.366	8.045	31.253	1.00	16.36
2862	O	TYR	A	201	-18.743	8.351	32.385	1.00	16.24
2863	N	SER	A	202	-18.297	8.921	30.258	1.00	17.53
2865	CA	SER	A	202	-18.686	10.314	30.468	1.00	19.44
2867	CB	SER	A	202	-18.355	11.181	29.255	1.00	19.61
2870	OG	SER	A	202	-18.724	12.536	29.491	1.00	22.68
2872	C	SER	A	202	-20.167	10.422	30.799	1.00	20.40
2873	O	SER	A	202	-20.544	11.153	31.711	1.00	21.05
2874	N	VAL	A	203	-21.007	9.695	30.070	1.00	21.19



# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
2876	CA	VAL	A	203	-22.453	9.794	30.294	1.00	21.92
2878	CB	VAL	A	203	-23.268	9.420	29.044	1.00	22.11
2880	CG1	VAL	A	203	-22.967	10.392	27.923	1.00	23.12
2884	CG2	VAL	A	203	-23.012	7.998	28.612	1.00	22.69
2888	C	VAL	A	203	-22.919	8.984	31.504	1.00	22.02
2889	O	VAL	A	203	-23.911	9.344	32.143	1.00	22.21
2890	N	SER	A	204	-22.189	7.921	31.841	1.00	21.78
2892	CA	SER	A	204	-22.536	7.056	32.967	1.00	22.12
2894	CB	BSER	A	204	-22.225	5.588	32.650	0.35	22.13
2895	CB	ASER	A	204	-22.186	5.600	32.657	0.65	22.30
2900	OG	BSER	A	204	-20.846	5.383	32.402	0.35	21.81
2901	OG	ASER	A	204	-22.758	5.185	31.430	0.65	22.86
2904	C	SER	A	204	-21.825	7.499	34.246	1.00	22.25
2905	O	SER	A	204	-21.966	6.860	35.283	1.00	22.52
2906	N	ARG	A	205	-21.071	8.596	34.155	1.00	22.50
2908	CA	ARG	A	205	-20.340	9.175	35.284	1.00	22.65
2910	CB	ARG	A	205	-21.320	9.885	36.227	1.00	23.63
2913	CG	ARG	A	205	-22.129	10.955	35.495	1.00	26.42
2916	CD	ARG	A	205	-22.691	12.073	36.368	1.00	30.05
2919	NE	ARG	A	205	-23.130	13.213	35.557	1.00	33.49
2921	CZ	ARG	A	205	-23.802	14.266	36.021	1.00	36.30
2922	NH1	ARG	A	205	-24.128	14.354	37.308	1.00	37.68
2925	NH2	ARG	A	205	-24.152	15.243	35.192	1.00	37.47
2928	C	ARG	A	205	-19.436	8.157	35.997	1.00	21.75
2929	O	ARG	A	205	-19.429	8.043	37.225	1.00	22.16
2930	N	VAL	A	206	-18.699	7.398	35.187	1.00	19.77
2932	CA	VAL	A	206	-17.629	6.521	35.636	1.00	18.53
2934	CB	VAL	A	206	-17.510	5.273	34.710	1.00	18.32
2936	CG1	VAL	A	206	-16.294	4.434	35.069	1.00	18.31
2940	CG2	VAL	A	206	-18.787	4.427	34.778	1.00	18.64
2944	C	VAL	A	206	-16.342	7.347	35.607	1.00	17.65
2945	O	VAL	A	206	-15.908	7.799	34.536	1.00	16.81
2946	N	ASN	A	207	-15.729	7.545	36.775	1.00	16.60
2948	CA	ASN	A	207	-14.577	8.449	36.912	1.00	16.29
2950	CB	BASN	A	207	-14.622	9.176	38.266	0.35	16.45
2951	CB	AASN	A	207	-14.604	9.166	38.264	0.65	16.92
2956	CG	BASN	A	207	-13.582	10.292	38.384	0.35	16.63
2957	CG	AASN	A	207	-15.857	9.996	38.459	0.65	18.02
2958	OD1	BASN	A	207	-13.182	10.663	39.490	0.35	18.02
2959	OD1	AASN	A	207	-16.218	10.807	37.606	0.65	20.91
2960	ND2	BASN	A	207	-13.150	10.834	37.253	0.35	16.67
2961	ND2	AASN	A	207	-16.529	9.798	39.589	0.65	20.96
2966	C	ASN	A	207	-13.267	7.691	36.742	1.00	15.34
2967	O	ASN	A	207	-12.395	7.690	37.617	1.00	15.45
2968	N	VAL	A	208	-13.158	7.030	35.597	1.00	14.20
2970	CA	VAL	A	208	-11.942	6.343	35.195	1.00	13.45
2972	CB	VAL	A	208	-12.183	4.834	35.064	1.00	13.22
2974	CG1	VAL	A	208	-10.943	4.118	34.514	1.00	13.60
2978	CG2	VAL	A	208	-12.592	4.249	36.418	1.00	13.16

## FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
2982	C	VAL	A	208	-11.505	6.942	33.871	1.00	12.86
2983	O	VAL	A	208	-12.270	6.951	32.912	1.00	13.43
2984	N	SER	A	209	-10.281	7.459	33.826	1.00	11.80
2986	CA	SER	A	209	-9.765	8.080	32.606	1.00	12.06
2988	CB	SER	A	209	-8.677	9.108	32.923	1.00	11.61
2991	OG	SER	A	209	-7.560	8.535	33.583	1.00	12.01
2993	C	SER	A	209	-9.226	7.029	31.658	1.00	11.87
2994	O	SER	A	209	-8.808	5.964	32.090	1.00	11.60
2995	N	ILE	A	210	-9.218	7.350	30.365	1.00	11.74
2997	CA	ILE	A	210	-8.645	6.501	29.326	1.00	12.08
2999	CB	ILE	A	210	-9.750	5.893	28.448	1.00	12.81
3001	CG1	ILE	A	210	-10.628	4.959	29.278	1.00	13.18
3004	CD1	ILE	A	210	-11.876	4.539	28.563	1.00	13.74
3008	CG2	ILE	A	210	-9.173	5.164	27.241	1.00	14.13
3012	C	ILE	A	210	-7.730	7.382	28.490	1.00	11.61
3013	O	ILE	A	210	-8.176	8.382	27.934	1.00	11.26
3014	N	THR	A	211	-6.464	6.992	28.398	1.00	11.71
3016	CA	THR	A	211	-5.444	7.714	27.653	1.00	11.63
3018	CB	THR	A	211	-4.251	8.069	28.580	1.00	12.61
3020	OG1	THR	A	211	-4.692	8.889	29.671	1.00	12.57
3022	CG2	THR	A	211	-3.212	8.896	27.852	1.00	13.19
3026	C	THR	A	211	-4.948	6.814	26.532	1.00	12.06
3027	O	THR	A	211	-4.465	5.723	26.810	1.00	12.41
3028	N	LEU	A	212	-5.064	7.270	25.288	1.00	11.47
3030	CA	LEU	A	212	-4.572	6.541	24.118	1.00	11.73
3032	CB	LEU	A	212	-5.599	6.573	22.985	1.00	11.89
3035	CG	LEU	A	212	-5.247	5.792	21.716	1.00	13.42
3037	CD1	LEU	A	212	-6.179	6.146	20.556	1.00	14.83
3041	CD2	LEU	A	212	-5.280	4.298	21.994	1.00	14.25
3045	C	LEU	A	212	-3.279	7.207	23.674	1.00	11.71
3046	O	LEU	A	212	-3.255	8.403	23.412	1.00	11.69
3047	N	CYS	A	213	-2.200	6.432	23.594	1.00	11.78
3049	CA	CYS	A	213	-0.899	6.986	23.257	1.00	12.57
3051	CB	CYS	A	213	0.158	6.442	24.214	1.00	12.33
3054	SG	CYS	A	213	-0.269	6.724	25.947	1.00	15.88
3055	C	CYS	A	213	-0.585	6.617	21.826	1.00	11.97
3056	O	CYS	A	213	-0.706	5.458	21.451	1.00	14.09
3057	N	VAL	A	214	-0.220	7.604	21.025	1.00	10.58
3059	CA	VAL	A	214	0.099	7.413	19.617	1.00	9.96
3061	CB	VAL	A	214	-0.691	8.407	18.758	1.00	9.46
3063	CG1	VAL	A	214	-0.307	8.283	17.279	1.00	11.00
3067	CG2	VAL	A	214	-2.199	8.211	18.965	1.00	11.02
3071	C	VAL	A	214	1.587	7.650	19.439	1.00	10.01
3072	O	VAL	A	214	2.042	8.791	19.547	1.00	10.72
3073	N	LEU	A	215	2.326	6.569	19.184	1.00	9.51
3075	CA	LEU	A	215	3.784	6.592	19.172	1.00	9.51
3077	CB	LEU	A	215	4.333	5.450	20.014	1.00	9.27
3080	CG	LEU	A	215	3.845	5.345	21.453	1.00	10.33
3082	CD1	LEU	A	215	4.611	4.249	22.149	1.00	10.27

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
3086	CD2	LEU	A	215	3.975	6.671	22.180	1.00	12.44
3090	C	LEU	A	215	4.361	6.478	17.768	1.00	9.30
3091	O	LEU	A	215	3.993	5.607	16.989	1.00	9.46
3092	N	GLY	A	216	5.305	7.354	17.481	1.00	9.64
3094	CA	GLY	A	216	6.161	7.204	16.325	1.00	9.54
3097	C	GLY	A	216	7.254	6.202	16.613	1.00	10.04
3098	O	GLY	A	216	7.137	5.367	17.517	1.00	9.95
3099	N	LEU	A	217	8.331	6.296	15.846	1.00	9.88
3101	CA	LEU	A	217	9.442	5.348	15.968	1.00	9.63
3103	CB	LEU	A	217	10.387	5.462	14.782	1.00	9.73
3106	CG	LEU	A	217	11.633	4.582	14.836	1.00	9.78
3108	CD1	LEU	A	217	11.287	3.105	14.786	1.00	11.38
3112	CD2	LEU	A	217	12.544	4.940	13.675	1.00	10.79
3116	C	LEU	A	217	10.209	5.573	17.254	1.00	9.53
3117	O	LEU	A	217	10.713	6.676	17.500	1.00	9.71
3118	N	ILE	A	218	10.292	4.521	18.064	1.00	9.84
3120	CA	ILE	A	218	10.954	4.544	19.367	1.00	10.10
3122	CB	ILE	A	218	9.973	4.157	20.509	1.00	10.68
3124	CG1	ILE	A	218	8.611	4.868	20.367	1.00	10.23
3127	CD1	ILE	A	218	8.679	6.406	20.385	1.00	10.45
3131	CG2	ILE	A	218	10.593	4.418	21.872	1.00	11.90
3135	C	ILE	A	218	12.102	3.542	19.306	1.00	10.59
3136	O	ILE	A	218	11.950	2.463	18.748	1.00	11.02
3137	N	ASP	A	219	13.239	3.882	19.904	1.00	10.63
3139	CA	ASP	A	219	14.461	3.072	19.734	1.00	10.92
3141	CB	ASP	A	219	15.698	3.950	19.938	1.00	11.57
3144	CG	ASP	A	219	15.847	4.431	21.346	1.00	12.72
3145	OD1	ASP	A	219	16.832	5.159	21.603	1.00	17.04
3146	OD2	ASP	A	219	15.067	4.157	22.263	1.00	13.80
3147	C	ASP	A	219	14.551	1.799	20.599	1.00	10.52
3148	O	ASP	A	219	15.630	1.428	21.088	1.00	11.55
3149	N	THR	A	220	13.445	1.079	20.730	1.00	10.56
3151	CA	THR	A	220	13.486	-0.234	21.356	1.00	10.32
3153	CB	THR	A	220	12.060	-0.775	21.601	1.00	10.52
3155	OG1	THR	A	220	11.409	-1.005	20.341	1.00	10.00
3157	CG2	THR	A	220	11.193	0.247	22.334	1.00	10.69
3161	C	THR	A	220	14.239	-1.232	20.480	1.00	10.14
3162	O	THR	A	220	14.325	-1.076	19.267	1.00	10.03
3163	N	GLU	A	221	14.783	-2.275	21.090	1.00	10.29
3165	CA	GLU	A	221	15.470	-3.321	20.324	1.00	11.82
3167	CB	GLU	A	221	15.967	-4.433	21.243	1.00	12.41
3170	CG	GLU	A	221	16.656	-5.585	20.515	1.00	17.63
3173	CD	GLU	A	221	17.681	-6.346	21.348	1.00	25.15
3174	OE1	GLU	A	221	17.473	-7.562	21.582	1.00	29.83
3175	OE2	GLU	A	221	18.719	-5.757	21.739	1.00	30.76
3176	C	GLU	A	221	14.581	-3.891	19.223	1.00	10.51
3177	O	GLU	A	221	15.037	-4.102	18.096	1.00	10.36
3178	N	THR	A	222	13.306	-4.125	19.537	1.00	10.29
3180	CA	THR	A	222	12.375	-4.592	18.538	1.00	10.08

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
3182	CB	THR	A	222	11.003	-4.767	19.175	1.00	10.12
3184	OG1	THR	A	222	11.080	-5.848	20.104	1.00	11.30
3186	CG2	THR	A	222	9.959	-5.155	18.136	1.00	11.15
3190	C	THR	A	222	12.304	-3.682	17.320	1.00	10.05
3191	O	THR	A	222	12.422	-4.148	16.189	1.00	10.05
3192	N	ALA	A	223	12.117	-2.382	17.540	1.00	10.23
3194	CA	ALA	A	223	12.030	-1.451	16.430	1.00	9.76
3196	CB	ALA	A	223	11.614	-0.088	16.901	1.00	9.78
3200	C	ALA	A	223	13.341	-1.373	15.654	1.00	9.93
3201	O	ALA	A	223	13.335	-1.310	14.432	1.00	10.36
3202	N	MET	A	224	14.455	-1.408	16.363	1.00	10.57
3204	CA	MET	A	224	15.745	-1.230	15.695	1.00	10.91
3206	CB	MET	A	224	16.828	-0.887	16.705	1.00	11.45
3209	CG	MET	A	224	16.596	0.451	17.424	1.00	11.79
3212	SD	MET	A	224	16.480	1.911	16.350	1.00	14.5
3213	CE	MET	A	224	14.771	1.998	15.995	1.00	15.91
3217	C	MET	A	224	16.098	-2.458	14.863	1.00	11.87
3218	O	MET	A	224	16.793	-2.355	13.857	1.00	11.83
3219	N	LYS	A	225	15.578	-3.613	15.251	1.00	12.68
3221	CA	LYS	A	225	15.725	-4.817	14.446	1.00	14.34
3223	CB	LYS	A	225	15.419	-6.052	15.302	1.00	14.91
3226	CG	LYS	A	225	16.580	-6.440	16.197	1.00	19.32
3229	CD	LYS	A	225	16.299	-7.717	16.970	1.00	24.07
3232	CE	LYS	A	225	17.430	-8.057	17.917	1.00	26.90
3235	NZ	LYS	A	225	18.628	-8.593	17.203	1.00	29.50
3239	C	LYS	A	225	14.814	-4.780	13.209	1.00	14.21
3240	O	LYS	A	225	15.182	-5.293	12.159	1.00	15.40
3241	N	ALA	A	226	13.642	-4.156	13.330	1.00	13.78
3243	CA	ALA	A	226	12.643	-4.146	12.258	1.00	13.40
3245	CB	ALA	A	226	11.256	-3.895	12.843	1.00	13.11
3249	C	ALA	A	226	12.910	-3.134	11.138	1.00	13.23
3250	O	ALA	A	226	12.699	-3.436	9.969	1.00	13.27
3251	N	VAL	A	227	13.356	-1.930	11.480	1.00	12.92
3253	CA	VAL	A	227	13.503	-0.868	10.476	1.00	13.22
3255	CB	VAL	A	227	13.304	0.552	11.076	1.00	13.18
3257	CG1	VAL	A	227	11.923	0.675	11.717	1.00	13.18
3261	CG2	VAL	A	227	14.424	0.921	12.046	1.00	14.17
3265	C	VAL	A	227	14.851	-0.965	9.737	1.00	13.49
3266	O	VAL	A	227	15.706	-1.784	10.090	1.00	13.51
3267	N	SER	A	228	15.012	-0.132	8.711	1.00	13.96
3269	CA	SER	A	228	16.142	-0.200	7.791	1.00	14.64
3271	CB	SER	A	228	15.655	-0.693	6.427	1.00	15.09
3274	OG	SER	A	228	16.690	-0.626	5.454	1.00	17.17
3276	C	SER	A	228	16.872	1.133	7.626	1.00	14.31
3277	O	SER	A	228	16.260	2.198	7.534	1.00	14.90
3278	N	GLY	A	229	18.196	1.067	7.586	1.00	14.06
3280	CA	GLY	A	229	19.010	2.186	7.148	1.00	13.99
3283	C	GLY	A	229	18.900	3.389	8.062	1.00	14.34
3284	O	GLY	A	229	18.809	3.241	9.281	1.00	13.98

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
3285	N	ILE	A	230	18.881	4.586	7.479	1.00	14.68
3287	CA	ILE	A	230	18.909	5.810	8.272	1.00	15.19
3289	CB	ILE	A	230	19.153	7.066	7.400	1.00	15.60
3291	CG1	ILE	A	230	18.015	7.295	6.402	1.00	16.97
3294	CD1	ILE	A	230	18.010	8.693	5.829	1.00	19.57
3298	CG2	ILE	A	230	20.492	6.976	6.696	1.00	16.66
3302	C	ILE	A	230	17.655	6.019	9.108	1.00	14.94
3303	O	ILE	A	230	17.651	6.870	9.989	1.00	15.39
3304	N	VAL	A	231	16.606	5.249	8.841	1.00	15.06
3306	CA	VAL	A	231	15.406	5.304	9.675	1.00	15.19
3308	CB	VAL	A	231	14.317	4.319	9.170	1.00	15.25
3310	CG1	VAL	A	231	13.105	4.285	10.119	1.00	15.04
3314	CG2	VAL	A	231	13.891	4.690	7.750	1.00	15.23
3318	C	VAL	A	231	15.768	5.040	11.137	1.00	15.39
3319	O	VAL	A	231	15.167	5.629	12.025	1.00	15.53
3320	N	HIS	A	232	16.748	4.170	11.390	1.00	15.81
3322	CA	HIS	A	232	17.231	3.918	12.757	1.00	16.19
3324	CB	HIS	A	232	18.475	3.018	12.782	1.00	15.89
3327	CG	HIS	A	232	18.254	1.631	12.249	1.00	14.26
3328	ND1	HIS	A	232	17.805	0.589	13.030	1.00	16.24
3330	CE1	HIS	A	232	17.730	-0.505	12.294	1.00	13.18
3332	NE2	HIS	A	232	18.122	-0.215	11.070	1.00	13.71
3334	CD2	HIS	A	232	18.458	1.112	11.018	1.00	10.97
3336	C	HIS	A	232	17.575	5.216	13.495	1.00	16.92
3337	O	HIS	A	232	17.352	5.321	14.694	1.00	18.81
3338	N	MET	A	233	18.127	6.192	12.781	1.00	17.36
3340	CA	MET	A	233	18.622	7.421	13.410	1.00	17.67
3342	CB	MET	A	233	19.733	8.021	12.547	1.00	18.33
3345	CG	MET	A	233	20.915	7.057	12.391	1.00	20.88
3348	SD	MET	A	233	22.408	7.841	11.894	1.00	26.90
3349	CE	MET	A	233	22.816	8.658	13.404	1.00	25.25
3353	C	MET	A	233	17.509	8.439	13.668	1.00	17.20
3354	O	MET	A	233	17.734	9.486	14.273	1.00	17.30
3355	N	GLN	A	234	16.306	8.104	13.226	1.00	16.57
3357	CA	GLN	A	234	15.149	8.973	13.327	1.00	16.31
3359	CB	GLN	A	234	14.430	8.974	11.973	1.00	17.11
3362	CG	GLN	A	234	15.384	9.358	10.831	1.00	17.53
3365	CD	GLN	A	234	14.822	9.234	9.417	1.00	19.66
3366	OE1	GLN	A	234	15.417	9.778	8.473	1.00	23.54
3367	NE2	GLN	A	234	13.717	8.538	9.254	1.00	18.05
3370	C	GLN	A	234	14.230	8.503	14.458	1.00	15.78
3371	O	GLN	A	234	13.066	8.894	14.510	1.00	16.20
3372	N	ALA	A	235	14.763	7.674	15.357	1.00	14.80
3374	CA	ALA	A	235	14.009	7.147	16.497	1.00	14.83
3376	CB	ALA	A	235	14.516	5.770	16.848	1.00	14.44
3380	C	ALA	A	235	14.104	8.048	17.713	1.00	14.74
3381	O	ALA	A	235	15.145	8.677	17.962	1.00	16.24
3382	N	ALA	A	236	13.027	8.100	18.486	1.00	12.99
3384	CA	ALA	A	236	12.997	8.819	19.751	1.00	12.70

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
3386	CB	ALA	A	236	11.606	9.349	20.015	1.00	12.97
3390	C	ALA	A	236	13.445	7.893	20.888	1.00	12.58
3391	O	ALA	A	236	13.287	6.676	20.801	1.00	12.11
3392	N	PRO	A	237	13.985	8.449	21.965	1.00	12.73
3393	CA	PRO	A	237	14.469	7.630	23.088	1.00	12.81
3395	CB	PRO	A	237	15.226	8.626	23.974	1.00	13.23
3398	CG	PRO	A	237	15.042	9.967	23.379	1.00	13.72
3401	CD	PRO	A	237	14.199	9.889	22.188	1.00	13.31
3404	C	PRO	A	237	13.360	6.949	23.884	1.00	12.51
3405	O	PRO	A	237	12.389	7.585	24.290	1.00	12.66
3406	N	LYS	A	238	13.513	5.654	24.113	1.00	11.91
3408	CA	LYS	A	238	12.494	4.887	24.831	1.00	11.86
3410	CB	LYS	A	238	12.829	3.389	24.808	1.00	12.07
3413	CG	LYS	A	238	14.183	3.006	25.404	1.00	12.85
3416	CD	LYS	A	238	14.478	1.541	25.156	1.00	13.91
3419	CE	LYS	A	238	15.728	1.099	25.895	1.00	15.43
3422	NZ	LYS	A	238	16.074	-0.331	25.644	1.00	17.83
3426	C	LYS	A	238	12.259	5.362	26.262	1.00	12.41
3427	O	LYS	A	238	11.145	5.262	26.772	1.00	12.64
3428	N	GLU	A	239	13.301	5.875	26.919	1.00	12.99
3430	CA	GLU	A	239	13.148	6.368	28.285	1.00	14.06
3432	CB	GLU	A	239	14.503	6.733	28.904	1.00	15.10
3435	CG	GLU	A	239	14.388	7.171	30.358	1.00	18.88
3438	CD	GLU	A	239	15.720	7.442	31.039	1.00	23.63
3439	OE1	GLU	A	239	15.780	8.402	31.834	1.00	27.51
3440	OE2	GLU	A	239	16.697	6.692	30.808	1.00	28.46
3441	C	GLU	A	239	12.226	7.575	28.318	1.00	13.62
3442	O	GLU	A	239	11.351	7.657	29.178	1.00	13.63
3443	N	GLU	A	240	12.406	8.500	27.380	1.00	13.23
3445	CA	GLU	A	240	11.571	9.704	27.321	1.00	13.79
3447	CB	GLU	A	240	12.157	10.747	26.353	1.00	14.47
3450	CG	GLU	A	240	11.373	12.055	26.303	1.00	18.33
3453	CD	GLU	A	240	12.038	13.136	25.454	1.00	22.78
3454	OE1	GLU	A	240	11.851	13.149	24.210	1.00	24.01
3455	OE2	GLU	A	240	12.755	13.987	26.031	1.00	26.83
3456	C	GLU	A	240	10.134	9.349	26.929	1.00	13.09
3457	O	GLU	A	240	9.168	9.859	27.509	1.00	12.73
3458	N	CYS	A	241	10.008	8.464	25.954	1.00	12.39
3460	CA	CYS	A	241	8.709	7.983	25.510	1.00	12.17
3462	CB	CYS	A	241	8.893	6.903	24.454	1.00	12.41
3465	SG	CYS	A	241	7.346	6.166	23.884	1.00	13.2
3466	C	CYS	A	241	7.901	7.441	26.677	1.00	11.60
3467	O	CYS	A	241	6.749	7.835	26.884	1.00	11.86
3468	N	ALA	A	242	8.517	6.552	27.445	1.00	11.18
3470	CA	ALA	A	242	7.882	5.954	28.624	1.00	11.17
3472	CB	ALA	A	242	8.838	4.954	29.306	1.00	11.30
3476	C	ALA	A	242	7.399	6.990	29.628	1.00	11.69
3477	O	ALA	A	242	6.306	6.880	30.158	1.00	12.03
3478	N	LEU	A	243	8.218	7.998	29.897	1.00	12.30

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
3480	CA	LEU	A	243	7.835	9.038	30.842	1.00	12.71
3482	CB	LEU	A	243	9.016	9.957	31.163	1.00	13.30
3485	CG	LEU	A	243	8.728	11.016	32.233	1.00	14.81
3487	CD1	LEU	A	243	8.259	10.409	33.534	1.00	17.02
3491	CD2	LEU	A	243	9.956	11.876	32.464	1.00	16.27
3495	C	LEU	A	243	6.641	9.837	30.323	1.00	12.58
3496	O	LEU	A	243	5.713	10.093	31.067	1.00	13.14
3497	N	GLU	A	244	6.634	10.181	29.041	1.00	12.66
3499	CA	GLU	A	244	5.509	10.933	28.475	1.00	13.16
3501	CB	GLU	A	244	5.800	11.388	27.042	1.00	13.53
3504	CG	GLU	A	244	6.884	12.456	26.905	1.00	15.47
3507	CD	GLU	A	244	6.668	13.672	27.802	1.00	18.14
3508	OE1	GLU	A	244	7.661	14.149	28.385	1.00	21.51
3509	OE2	GLU	A	244	5.520	14.166	27.928	1.00	20.54
3510	C	GLU	A	244	4.191	10.145	28.522	1.00	12.61
3511	O	GLU	A	244	3.115	10.729	28.712	1.00	13.71
3512	N	ILE	A	245	4.268	8.827	28.374	1.00	12.09
3514	CA	ILE	A	245	3.086	7.972	28.501	1.00	11.82
3516	CB	ILE	A	245	3.400	6.522	28.110	1.00	11.22
3518	CG1	ILE	A	245	3.666	6.437	26.607	1.00	11.30
3521	CD1	ILE	A	245	4.237	5.125	26.206	1.00	10.91
3525	CG2	ILE	A	245	2.237	5.596	28.474	1.00	11.57
3529	C	ILE	A	245	2.562	8.033	29.936	1.00	12.26
3530	O	ILE	A	245	1.370	8.235	30.145	1.00	11.84
3531	N	ILE	A	246	3.452	7.881	30.910	1.00	12.36
3533	CA	ILE	A	246	3.061	7.944	32.321	1.00	12.96
3535	CB	ILE	A	246	4.256	7.606	33.245	1.00	13.20
3537	CG1	ILE	A	246	4.616	6.114	33.116	1.00	13.37
3540	CD1	ILE	A	246	6.015	5.764	33.620	1.00	13.81
3544	CG2	ILE	A	246	3.939	7.962	34.694	1.00	13.32
3548	C	ILE	A	246	2.471	9.317	32.663	1.00	13.52
3549	O	ILE	A	246	1.467	9.400	33.376	1.00	14.24
3550	N	LYS	A	247	3.094	10.383	32.164	1.00	13.79
3552	CA	LYS	A	247	2.634	11.744	32.454	1.00	14.92
3554	CB	LYS	A	247	3.561	12.782	31.834	1.00	15.40
3557	CG	LYS	A	247	4.929	12.946	32.496	1.00	18.06
3560	CD	LYS	A	247	5.528	14.312	32.153	1.00	22.18
3563	CE	LYS	A	247	6.996	14.233	31.799	1.00	24.53
3566	NZ	LYS	A	247	7.476	15.495	31.166	1.00	24.96
3570	C	LYS	A	247	1.220	11.944	31.916	1.00	14.92
3571	O	LYS	A	247	0.358	12.487	32.609	1.00	14.25
3572	N	GLY	A	248	0.987	11.495	30.685	1.00	14.56
3574	CA	GLY	A	248	-0.323	11.566	30.064	1.00	14.78
3577	C	GLY	A	248	-1.385	10.851	30.873	1.00	14.66
3578	O	GLY	A	248	-2.468	11.383	31.084	1.00	15.08
3579	N	GLY	A	249	-1.078	9.641	31.326	1.00	14.70
3581	CA	GLY	A	249	-1.990	8.881	32.153	1.00	14.83
3584	C	GLY	A	249	-2.277	9.551	33.486	1.00	14.79
3585	O	GLY	A	249	-3.432	9.624	33.905	1.00	15.25

## FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
3586	N	ALA	A	250	-1.233	10.037	34.150	1.00	14.46
3588	CA	ALA	A	250	-1.383	10.697	35.450	1.00	14.16
3590	CB	ALA	A	250	-0.026	11.039	36.026	1.00	14.16
3594	C	ALA	A	250	-2.241	11.948	35.352	1.00	14.08
3595	O	ALA	A	250	-3.025	12.241	36.265	1.00	14.84
3596	N	LEU	A	251	-2.101	12.681	34.249	1.00	13.91
3598	CA	LEU	A	251	-2.840	13.928	34.031	1.00	14.09
3600	CB	LEU	A	251	-2.024	14.891	33.156	1.00	14.26
3603	CG	LEU	A	251	-0.724	15.384	33.794	1.00	15.23
3605	CD1	LEU	A	251	0.090	16.174	32.789	1.00	16.39
3609	CD2	LEU	A	251	-1.010	16.207	35.036	1.00	16.11
3613	C	LEU	A	251	-4.211	13.680	33.397	1.00	13.99
3614	O	LEU	A	251	-4.947	14.627	33.113	1.00	14.70
3615	N	ARG	A	252	-4.546	12.413	33.161	1.00	13.35
3617	CA	ARG	A	252	-5.861	12.021	32.657	1.00	13.70
3619	CB	ARG	A	252	-6.947	12.389	33.678	1.00	13.81
3622	CG	ARG	A	252	-6.669	11.842	35.062	1.00	13.84
3625	CD	ARG	A	252	-7.733	12.183	36.087	1.00	13.80
3628	NE	ARG	A	252	-8.904	11.295	36.082	1.00	13.43
3630	CZ	ARG	A	252	-8.958	10.089	36.647	1.00	13.38
3631	NH1	ARG	A	252	-7.903	9.566	37.267	1.00	13.53
3634	NH2	ARG	A	252	-10.092	9.397	36.601	1.00	14.15
3637	C	ARG	A	252	-6.151	12.625	31.265	1.00	14.05
3638	O	ARG	A	252	-7.292	12.949	30.924	1.00	13.82
3639	N	GLN	A	253	-5.096	12.772	30.463	1.00	14.24
3641	CA	GLN	A	253	-5.219	13.221	29.084	1.00	14.68
3643	CB	GLN	A	253	-3.841	13.537	28.488	1.00	15.44
3646	CG	GLN	A	253	-3.119	14.683	29.126	1.00	18.33
3649	CD	GLN	A	253	-1.741	14.927	28.502	1.00	18.88
3650	OE1	GLN	A	253	-1.439	14.439	27.399	1.00	24.01
3651	NE2	GLN	A	253	-0.919	15.675	29.195	1.00	23.09
3654	C	GLN	A	253	-5.893	12.160	28.221	1.00	14.73
3655	O	GLN	A	253	-5.687	10.960	28.419	1.00	14.76
3656	N	GLU	A	254	-6.691	12.593	27.257	1.00	14.58
3658	CA	GLU	A	254	-7.359	11.641	26.376	1.00	14.78
3660	CB	GLU	A	254	-8.500	12.296	25.619	1.00	15.34
3663	CG	GLU	A	254	-9.619	12.674	26.572	1.00	18.01
3666	CD	GLU	A	254	-10.911	13.085	25.905	1.00	21.86
3667	OE1	GLU	A	254	-11.774	13.602	26.638	1.00	25.73
3668	OE2	GLU	A	254	-11.082	12.878	24.685	1.00	23.79
3669	C	GLU	A	254	-6.350	10.996	25.434	1.00	14.10
3670	O	GLU	A	254	-6.396	9.805	25.203	1.00	12.59
3671	N	GLU	A	255	-5.431	11.786	24.902	1.00	14.29
3673	CA	GLU	A	255	-4.430	11.253	23.984	1.00	14.94
3675	CB	GLU	A	255	-4.854	11.456	22.514	1.00	15.32
3678	CG	GLU	A	255	-6.153	10.719	22.161	1.00	17.27
3681	CD	GLU	A	255	-6.493	10.670	20.673	1.00	20.11
3682	OE1	GLU	A	255	-7.174	9.689	20.251	1.00	22.21
3683	OE2	GLU	A	255	-6.133	11.613	19.931	1.00	21.72



# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
3684	C	GLU	A	255	-3.058	11.858	24.242	1.00	15.03
3685	O	GLU	A	255	-2.938	13.016	24.660	1.00	16.89
3686	N	VAL	A	256	-2.040	11.039	24.028	1.00	14.51
3688	CA	VAL	A	256	-0.643	11.451	24.046	1.00	14.15
3690	CB	VAL	A	256	0.154	10.654	25.100	1.00	13.96
3692	CG1	VAL	A	256	1.649	10.938	24.997	1.00	15.69
3696	CG2	VAL	A	256	-0.363	10.939	26.515	1.00	14.47
3700	C	VAL	A	256	-0.079	11.170	22.659	1.00	13.85
3701	O	VAL	A	256	-0.284	10.094	22.106	1.00	14.72
3702	N	TYR	A	257	0.604	12.145	22.086	1.00	12.90
3704	CA	TYR	A	257	1.284	11.965	20.819	1.00	12.32
3706	CB	TYR	A	257	0.776	12.965	19.781	1.00	12.68
3709	CG	TYR	A	257	-0.619	12.658	19.299	1.00	13.34
3710	CD1	TYR	A	257	-1.729	13.026	20.043	1.00	17.02
3712	CE1	TYR	A	257	-3.020	12.734	19.601	1.00	16.67
3714	CZ	TYR	A	257	-3.186	12.041	18.417	1.00	16.83
3715	OH	TYR	A	257	-4.453	11.728	17.964	1.00	18.33
3717	CE2	TYR	A	257	-2.096	11.652	17.672	1.00	15.55
3719	CD2	TYR	A	257	-0.817	11.954	18.119	1.00	15.03
3721	C	TYR	A	257	2.764	12.178	21.076	1.00	12.67
3722	O	TYR	A	257	3.159	13.207	21.635	1.00	12.40
3723	N	TYR	A	258	3.574	11.195	20.695	1.00	12.14
3725	CA	TYR	A	258	5.012	11.228	20.957	1.00	12.17
3727	CB	TYR	A	258	5.382	10.400	22.194	1.00	12.26
3730	CG	TYR	A	258	6.847	10.529	22.532	1.00	12.49
3731	CD1	TYR	A	258	7.761	9.585	22.087	1.00	13.64
3733	CE1	TYR	A	258	9.085	9.706	22.351	1.00	14.93
3735	CZ	TYR	A	258	9.552	10.781	23.061	1.00	15.74
3736	OH	TYR	A	258	10.899	10.886	23.312	1.00	18.74
3738	CE2	TYR	A	258	8.678	11.756	23.507	1.00	15.65
3740	CD2	TYR	A	258	7.325	11.623	23.235	1.00	14.56
3742	C	TYR	A	258	5.811	10.766	19.741	1.00	12.04
3743	O	TYR	A	258	5.584	9.686	19.190	1.00	12.46
3744	N	ASP	A	259	6.746	11.613	19.332	1.00	11.98
3746	CA	ASP	A	259	7.596	11.362	18.189	1.00	12.06
3748	CB	ASP	A	259	6.877	11.734	16.890	1.00	12.28
3751	CG	ASP	A	259	7.592	11.199	15.662	1.00	12.82
3752	OD1	ASP	A	259	8.255	11.972	14.928	1.00	13.50
3753	OD2	ASP	A	259	7.567	9.997	15.367	1.00	13.61
3754	C	ASP	A	259	8.871	12.199	18.309	1.00	12.75
3755	O	ASP	A	259	8.907	13.196	19.023	1.00	14.17
3756	N	SER	A	260	9.915	11.803	17.593	1.00	12.69
3758	CA	SER	A	260	11.133	12.606	17.553	1.00	12.78
3760	CB	SER	A	260	12.245	11.818	16.859	1.00	13.14
3763	OG	SER	A	260	11.902	11.533	15.525	1.00	14.29
3765	C	SER	A	260	10.946	13.983	16.882	1.00	12.78
3766	O	SER	A	260	11.763	14.883	17.090	1.00	13.36
3767	N	SER	A	261	9.891	14.148	16.086	1.00	12.92
3769	CA	SER	A	261	9.662	15.385	15.342	1.00	13.13

## FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
3771	CB	SER	A	261	9.726	15.110	13.847	1.00	13.52
3774	OG	SER	A	261	9.558	16.314	13.106	1.00	15.49
3776	C	SER	A	261	8.316	16.047	15.645	1.00	12.86
3777	O	SER	A	261	7.282	15.391	15.669	1.00	12.36
3778	N	LEU	A	262	8.345	17.365	15.810	1.00	13.43
3780	CA	LEU	A	262	7.111	18.146	15.922	1.00	13.79
3782	CB	LEU	A	262	7.411	19.585	16.344	1.00	14.71
3785	CG	LEU	A	262	7.796	19.741	17.812	1.00	16.69
3787	CD1	LEU	A	262	8.483	21.061	18.024	1.00	18.30
3791	CD2	LEU	A	262	6.575	19.622	18.706	1.00	18.44
3795	C	LEU	A	262	6.295	18.149	14.632	1.00	13.50
3796	O	LEU	A	262	5.077	18.334	14.671	1.00	13.90
3797	N	TRP	A	263	6.940	17.954	13.485	1.00	12.96
3799	CA	TRP	A	263	6.191	17.805	12.251	1.00	12.95
3801	CB	TRP	A	263	7.105	17.575	11.054	1.00	13.21
3804	CG	TRP	A	263	7.833	18.797	10.591	1.00	13.06
3805	CD1	TRP	A	263	8.963	19.336	11.132	1.00	13.15
3807	NE1	TRP	A	263	9.358	20.436	10.409	1.00	13.91
3809	CE2	TRP	A	263	8.471	20.632	9.382	1.00	13.01
3810	CD2	TRP	A	263	7.497	19.615	9.469	1.00	12.54
3811	CE3	TRP	A	263	6.470	19.589	8.517	1.00	13.69
3813	CZ3	TRP	A	263	6.448	20.570	7.525	1.00	14.28
3815	CH2	TRP	A	263	7.422	21.570	7.475	1.00	14.58
3817	CZ2	TRP	A	263	8.441	21.625	8.389	1.00	14.67
3819	C	TRP	A	263	5.202	16.647	12.387	1.00	12.67
3820	O	TRP	A	263	4.068	16.737	11.925	1.00	13.16
3821	N	THR	A	264	5.631	15.575	13.048	1.00	12.43
3823	CA	THR	A	264	4.772	14.414	13.260	1.00	12.40
3825	CB	THR	A	264	5.601	13.208	13.720	1.00	12.33
3827	OG1	THR	A	264	6.631	12.927	12.761	1.00	13.89
3829	CG2	THR	A	264	4.745	11.949	13.762	1.00	13.45
3833	C	THR	A	264	3.675	14.672	14.275	1.00	12.94
3834	O	THR	A	264	2.493	14.489	13.973	1.00	13.32
3835	N	THR	A	265	4.044	15.080	15.488	1.00	12.88
3837	CA	THR	A	265	3.043	15.176	16.542	1.00	13.43
3839	CB	THR	A	265	3.653	15.379	17.924	1.00	13.61
3841	OG1	THR	A	265	4.476	16.544	17.950	1.00	13.50
3843	CG2	THR	A	265	4.581	14.223	18.285	1.00	14.31
3847	C	THR	A	265	2.030	16.277	16.270	1.00	13.30
3848	O	THR	A	265	0.882	16.148	16.656	1.00	14.73
3849	N	LEU	A	266	2.439	17.346	15.595	1.00	13.38
3851	CA	LEU	A	266	1.478	18.412	15.285	1.00	13.34
3853	CB	LEU	A	266	2.175	19.760	15.049	1.00	13.45
3856	CG	LEU	A	266	2.923	20.354	16.251	1.00	14.57
3858	CD1	LEU	A	266	3.639	21.633	15.849	1.00	14.76
3862	CD2	LEU	A	266	1.997	20.630	17.449	1.00	16.72
3866	C	LEU	A	266	0.573	18.063	14.107	1.00	13.75
3867	O	LEU	A	266	-0.626	18.331	14.158	1.00	14.43
3868	N	LEU	A	267	1.117	17.479	13.045	1.00	13.89

## FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
3870	CA	LEU	A	267	0.325	17.246	11.835	1.00	14.09
3872	CB	LEU	A	267	1.210	17.160	10.583	1.00	14.83
3875	CG	LEU	A	267	1.934	18.451	10.207	1.00	15.97
3877	CD1	LEU	A	267	2.932	18.187	9.095	1.00	16.94
3881	CD2	LEU	A	267	0.954	19.541	9.797	1.00	18.16
3885	C	LEU	A	267	-0.557	16.008	11.918	1.00	14.25
3886	O	LEU	A	267	-1.567	15.928	11.219	1.00	13.84
3887	N	ILE	A	268	-0.189	15.039	12.758	1.00	14.62
3889	CA	ILE	A	268	-0.932	13.783	12.823	1.00	15.29
3891	CB	ILE	A	268	-0.044	12.644	13.406	1.00	15.57
3893	CG1	ILE	A	268	-0.572	11.270	12.972	1.00	18.61
3896	CD1	ILE	A	268	-0.268	10.952	11.536	1.00	20.22
3900	CG2	ILE	A	268	0.071	12.769	14.928	1.00	16.48
3904	C	ILE	A	268	-2.228	13.949	13.625	1.00	15.51
3905	O	ILE	A	268	-3.153	13.132	13.514	1.00	15.43
3906	N	ARG	A	269	-2.306	14.995	14.444	1.00	15.82
3908	CA	ARG	A	269	-3.547	15.260	15.167	1.00	16.27
3910	CB	ARG	A	269	-3.358	16.396	16.173	1.00	17.51
3913	CG	ARG	A	269	-2.544	15.963	17.385	1.00	21.13
3916	CD	ARG	A	269	-2.787	16.788	18.636	1.00	26.97
3919	NE	ARG	A	269	-1.784	16.495	19.660	1.00	31.40
3921	CZ	ARG	A	269	-1.731	17.060	20.860	1.00	34.49
3922	NH1	ARG	A	269	-0.755	16.721	21.698	1.00	36.54
3925	NH2	ARG	A	269	-2.641	17.955	21.233	1.00	36.22
3928	C	ARG	A	269	-4.703	15.553	14.207	1.00	15.45
3929	O	ARG	A	269	-4.535	16.209	13.184	1.00	15.18
3930	N	ASN	A	270	-5.875	15.021	14.544	1.00	14.09
3932	CA	ASN	A	270	-7.104	15.241	13.782	1.00	13.41
3934	CB	ASN	A	270	-7.590	13.872	13.270	1.00	13.09
3937	CG	ASN	A	270	-8.893	13.927	12.462	1.00	13.39
3938	OD1	ASN	A	270	-9.536	12.880	12.232	1.00	13.86
3939	ND2	ASN	A	270	-9.261	15.110	11.992	1.00	13.50
3942	C	ASN	A	270	-8.148	15.912	14.688	1.00	13.21
3943	O	ASN	A	270	-9.079	15.250	15.128	1.00	12.55
3944	N	PRO	A	271	-7.996	17.206	14.995	1.00	13.34
3945	CA	PRO	A	271	-8.950	17.903	15.877	1.00	13.52
3947	CB	PRO	A	271	-8.372	19.327	15.969	1.00	13.91
3950	CG	PRO	A	271	-7.529	19.468	14.753	1.00	13.93
3953	CD	PRO	A	271	-6.916	18.111	14.553	1.00	13.66
3956	C	PRO	A	271	-10.378	17.921	15.331	1.00	13.69
3957	O	PRO	A	271	-11.315	17.977	16.131	1.00	13.14
3958	N	SER	A	272	-10.548	17.822	14.016	1.00	13.03
3960	CA	SER	A	272	-11.885	17.781	13.433	1.00	13.46
3962	CB	SER	A	272	-11.828	17.710	11.912	1.00	14.11
3965	OG	SER	A	272	-11.399	18.963	11.391	1.00	17.11
3967	C	SER	A	272	-12.707	16.612	13.937	1.00	13.00
3968	O	SER	A	272	-13.921	16.728	14.067	1.00	13.00
3969	N	ARG	A	273	-12.068	15.474	14.176	1.00	12.78
3971	CA	ARG	A	273	-12.801	14.324	14.697	1.00	11.90

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
3973	CB	ARG	A	273	-11.881	13.097	14.830	1.00	11.99
3976	CG	ARG	A	273	-12.475	11.991	15.640	1.00	11.46
3979	CD	ARG	A	273	-11.762	10.657	15.526	1.00	11.09
3982	NE	ARG	A	273	-11.980	9.902	16.767	1.00	9.70
3984	CZ	ARG	A	273	-11.256	8.861	17.148	1.00	9.95
3985	NH1	ARG	A	273	-10.316	8.378	16.366	1.00	9.89
3988	NH2	ARG	A	273	-11.483	8.314	18.321	1.00	10.33
3991	C	ARG	A	273	-13.461	14.652	16.049	1.00	12.29
3992	O	ARG	A	273	-14.641	14.399	16.232	1.00	11.23
3993	N	LYS	A	274	-12.712	15.206	16.994	1.00	13.15
3995	CA	LYS	A	274	-13.276	15.476	18.318	1.00	14.18
3997	CB	LYS	A	274	-12.195	15.840	19.347	1.00	15.51
4000	CG	LYS	A	274	-11.587	14.602	20.043	1.00	19.22
4003	CD	LYS	A	274	-12.529	13.934	21.064	1.00	23.59
4006	CE	LYS	A	274	-12.715	14.754	22.349	1.00	26.53
4009	NZ	LYS	A	274	-11.450	15.070	23.056	1.00	29.55
4013	C	LYS	A	274	-14.349	16.566	18.238	1.00	13.43
4014	O	LYS	A	274	-15.331	16.505	18.959	1.00	13.79
4015	N	ILE	A	275	-14.170	17.531	17.341	1.00	12.90
4017	CA	ILE	A	275	-15.179	18.569	17.120	1.00	12.53
4019	CB	ILE	A	275	-14.676	19.649	16.129	1.00	13.20
4021	CG1	ILE	A	275	-13.619	20.505	16.827	1.00	14.01
4024	CD1	ILE	A	275	-12.753	21.320	15.876	1.00	14.59
4028	CG2	ILE	A	275	-15.841	20.530	15.635	1.00	13.51
4032	C	ILE	A	275	-16.485	17.949	16.643	1.00	12.40
4033	O	ILE	A	275	-17.547	18.253	17.186	1.00	11.97
4034	N	LEU	A	276	-16.408	17.084	15.638	1.00	11.93
4036	CA	LEU	A	276	-17.606	16.459	15.099	1.00	12.46
4038	CB	LEU	A	276	-17.296	15.720	13.804	1.00	13.18
4041	CG	LEU	A	276	-16.908	16.625	12.636	1.00	15.33
4043	CD1	LEU	A	276	-16.447	15.767	11.453	1.00	17.19
4047	CD2	LEU	A	276	-18.057	17.527	12.230	1.00	16.58
4051	C	LEU	A	276	-18.252	15.529	16.115	1.00	11.71
4052	O	LEU	A	276	-19.473	15.491	16.220	1.00	12.57
4053	N	GLU	A	277	-17.451	14.796	16.881	1.00	11.42
4055	CA	GLU	A	277	-18.011	13.963	17.941	1.00	11.20
4057	CB	GLU	A	277	-16.933	13.172	18.678	1.00	11.21
4060	CG	GLU	A	277	-16.283	12.100	17.818	1.00	10.62
4063	CD	GLU	A	277	-15.046	11.474	18.436	1.00	11.45
4064	OE1	GLU	A	277	-14.485	10.547	17.821	1.00	10.82
4065	OE2	GLU	A	277	-14.594	11.890	19.531	1.00	13.35
4066	C	GLU	A	277	-18.805	14.818	18.920	1.00	11.99
4067	O	GLU	A	277	-19.901	14.453	19.318	1.00	12.45
4068	N	PHE	A	278	-18.271	15.981	19.265	1.00	12.15
4070	CA	PHE	A	278	-18.962	16.883	20.177	1.00	12.91
4072	CB	PHE	A	278	-18.035	18.014	20.619	1.00	13.16
4075	CG	PHE	A	278	-18.741	19.104	21.367	1.00	16.16
4076	CD1	PHE	A	278	-19.067	18.946	22.707	1.00	18.86
4078	CE1	PHE	A	278	-19.743	19.953	23.398	1.00	20.15

## FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
4080	CZ	PHE	A	278	-20.100	21.115	22.743	1.00	20.75
4082	CE2	PHE	A	278	-19.790	21.280	21.397	1.00	19.66
4084	CD2	PHE	A	278	-19.109	20.268	20.717	1.00	18.31
4086	C	PHE	A	278	-20.247	17.436	19.559	1.00	12.91
4087	O	PHE	A	278	-21.299	17.443	20.207	1.00	12.84
4088	N	LEU	A	279	-20.170	17.881	18.305	1.00	13.02
4090	CA	LEU	A	279	-21.320	18.473	17.626	1.00	13.85
4092	CB	LEU	A	279	-20.904	19.092	16.294	1.00	13.50
4095	CG	LEU	A	279	-20.063	20.361	16.453	1.00	13.69
4097	CD1	LEU	A	279	-19.497	20.792	15.115	1.00	13.87
4101	CD2	LEU	A	279	-20.866	21.492	17.087	1.00	14.19
4105	C	LEU	A	279	-22.418	17.434	17.418	1.00	15.13
4106	O	LEU	A	279	-23.612	17.754	17.490	1.00	14.67
4107	N	TYR	A	280	-22.009	16.187	17.206	1.00	17.39
4109	CA	TYR	A	280	-22.956	15.098	16.952	1.00	18.83
4111	CB	TYR	A	280	-22.263	13.922	16.248	1.00	18.64
4114	CG	TYR	A	280	-21.829	14.138	14.812	1.00	17.60
4115	CD1	TYR	A	280	-21.223	13.107	14.108	1.00	16.54
4117	CE1	TYR	A	280	-20.829	13.255	12.805	1.00	17.67
4119	CZ	TYR	A	280	-20.983	14.465	12.177	1.00	16.80
4120	OH	TYR	A	280	-20.580	14.601	10.870	1.00	19.36
4122	CE2	TYR	A	280	-21.584	15.517	12.844	1.00	16.35
4124	CD2	TYR	A	280	-22.003	15.351	14.163	1.00	16.97
4126	C	TYR	A	280	-23.625	14.583	18.236	1.00	20.92
4127	O	TYR	A	280	-24.668	13.909	18.160	1.00	22.66
4128	N	SER	A	281	-23.053	14.909	19.393	1.00	22.74
4130	CA	SER	A	281	-23.441	14.319	20.679	1.00	24.99
4132	CB	SER	A	281	-22.385	14.609	21.742	1.00	25.16
4135	OG	SER	A	281	-22.373	15.981	22.104	1.00	24.47
4137	C	SER	A	281	-24.806	14.743	21.222	1.00	27.70
4138	O	SER	A	281	-25.362	14.054	22.089	1.00	28.32
4139	N	THR	A	282	-25.330	15.867	20.748	1.00	30.09
4141	CA	THR	A	282	-26.631	16.359	21.220	1.00	32.53
4143	CB	THR	A	282	-26.808	17.861	20.901	1.00	32.60
4145	OG1	THR	A	282	-26.678	18.084	19.490	1.00	34.49
4147	CG2	THR	A	282	-25.699	18.699	21.521	1.00	34.08
4151	C	THR	A	282	-27.795	15.586	20.609	1.00	33.55
4152	O	THR	A	282	-28.919	15.684	21.096	1.00	33.93
4153	N	SER	A	283	-27.519	14.815	19.555	1.00	34.90
4155	CA	SER	A	283	-28.562	14.185	18.748	1.00	35.89
4157	CB	SER	A	283	-28.139	14.181	17.273	1.00	35.89
4160	OG	SER	A	283	-28.175	15.496	16.740	1.00	37.27
4162	C	SER	A	283	-28.970	12.770	19.189	1.00	36.40
4163	O	SER	A	283	-29.809	12.149	18.535	1.00	37.07
4164	N	TYR	A	284	-28.410	12.250	20.282	1.00	37.17
4166	CA	TYR	A	284	-28.940	10.995	20.839	1.00	37.25
4168	CB	BTYR	A	284	-27.988	9.804	20.643	0.35	37.05
4169	CB	ATYR	A	284	-28.006	9.802	20.558	0.65	37.18
4174	CG	BTYR	A	284	-26.677	10.145	19.995	0.35	35.02

## FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
4175	CG	ATYR	A	284	-26.519	10.087	20.631	0.65	35.41
4176	CD1BTYR	A	284		-26.531	10.078	18.617	0.35	33.54
4177	CD1ATYR	A	284		-25.709	10.016	19.495	0.65	34.19
4180	CE1BTYR	A	284		-25.339	10.385	18.013	0.35	32.28
4181	CE1ATYR	A	284		-24.334	10.270	19.576	0.65	33.47
4184	CZ	BTYR	A	284	-24.264	10.772	18.785	0.35	31.47
4185	CZ	ATYR	A	284	-23.774	10.592	20.800	0.65	32.46
4186	OH	BTYR	A	284	-23.086	11.080	18.172	0.35	30.12
4187	OH	ATYR	A	284	-22.428	10.845	20.910	0.65	31.11
4190	CE2BTYR	A	284		-24.374	10.846	20.161	0.35	31.97
4191	CE2ATYR	A	284		-24.562	10.664	21.930	0.65	33.01
4194	CD2BTYR	A	284		-25.580	10.531	20.760	0.35	33.31
4195	CD2ATYR	A	284		-25.921	10.411	21.839	0.65	33.91
4198	C	TYR	A	284	-29.307	11.115	22.319	1.00	38.54
4199	O	TYR	A	284	-28.651	11.823	23.089	1.00	39.00
4200	N	ASN	A	285	-30.371	10.404	22.683	1.00	39.93
4202	CA	ASN	A	285	-31.023	10.518	23.979	1.00	41.06
4204	CB	ASN	A	285	-32.547	10.472	23.792	1.00	41.26
4207	CG	ASN	A	285	-33.325	10.766	25.074	1.00	42.39
4208	OD1	ASN	A	285	-34.551	10.913	25.039	1.00	43.71
4209	ND2	ASN	A	285	-32.626	10.842	26.203	1.00	43.32
4212	C	ASN	A	285	-30.557	9.363	24.852	1.00	41.84
4213	O	ASN	A	285	-30.951	8.211	24.635	1.00	41.55
4214	N	MET	A	286	-29.717	9.681	25.835	1.00	43.04
4216	CA	MET	A	286	-29.148	8.662	26.719	1.00	43.94
4218	CB	MET	A	286	-27.654	8.322	26.524	1.00	44.34
4221	CG	MET	A	286	-26.829	9.341	25.747	1.00	45.83
4224	SD	MET	A	286	-25.780	8.554	24.522	1.00	49.97
4225	CE	MET	A	286	-24.522	7.957	25.487	1.00	48.62
4229	C	MET	A	286	-29.820	8.056	27.966	1.00	44.23
4230	O	MET	A	286	-29.294	7.130	28.584	1.00	44.03
4231	N	ASP	A	287	-30.963	8.648	28.327	1.00	44.71
4233	CA	ASP	A	287	-31.698	8.327	29.557	1.00	45.18
4235	CB	ASP	A	287	-33.059	9.048	29.574	1.00	45.46
4238	CG	ASP	A	287	-32.983	10.457	30.157	1.00	46.78
4239	OD1	ASP	A	287	-31.896	10.876	30.622	1.00	48.76
4240	OD2	ASP	A	287	-33.976	11.219	30.196	1.00	48.42
4241	C	ASP	A	287	-31.924	6.832	29.722	1.00	45.05
4242	O	ASP	A	287	-31.774	6.290	30.818	1.00	45.16
4243	N	ARG	A	288	-32.305	6.190	28.621	1.00	44.98
4245	CA	ARG	A	288	-32.384	4.733	28.511	1.00	45.09
4247	CB	ARG	A	288	-32.289	4.344	27.029	1.00	45.17
4250	CG	ARG	A	288	-33.171	3.189	26.602	1.00	45.72
4253	CD	ARG	A	288	-34.168	3.567	25.523	1.00	45.90
4256	NE	ARG	A	288	-34.313	2.539	24.499	1.00	46.47
4258	CZ	ARG	A	288	-35.102	2.654	23.438	1.00	46.36
4259	NH1	ARG	A	288	-35.822	3.755	23.253	1.00	46.20
4262	NH2	ARG	A	288	-35.177	1.664	22.558	1.00	46.85
4265	C	ARG	A	288	-31.259	4.017	29.265	1.00	45.02

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
4266	O	ARG	A	288	-31.488	3.024	29.958	1.00	44.94
4267	N	PHE	A	289	-30.042	4.527	29.088	1.00	44.85
4269	CA	PHE	A	289	-28.837	3.962	29.681	1.00	44.69
4271	CB	PHE	A	289	-27.821	3.652	28.579	1.00	44.59
4274	CG	PHE	A	289	-28.433	3.138	27.301	1.00	44.14
4275	CD1	PHE	A	289	-28.731	4.004	26.258	1.00	44.11
4277	CE1	PHE	A	289	-29.285	3.526	25.065	1.00	43.59
4279	CZ	PHE	A	289	-29.538	2.173	24.914	1.00	43.54
4281	CE2	PHE	A	289	-29.238	1.298	25.949	1.00	43.76
4283	CD2	PHE	A	289	-28.686	1.784	27.133	1.00	43.87
4285	C	PHE	A	289	-28.210	4.930	30.684	1.00	44.78
4286	O	PHE	A	289	-28.774	5.212	31.741	1.00	44.82
4287	N	GLN	B	20	-5.719	3.636	-4.824	1.00	36.45
4289	CA	GLN	B	20	-5.585	3.373	-6.276	1.00	35.95
4291	CB	GLN	B	20	-6.503	2.214	-6.665	1.00	35.41
4294	CG	GLN	B	20	-7.985	2.459	-6.412	1.00	31.81
4297	CD	GLN	B	20	-8.514	1.877	-5.103	1.00	27.25
4298	OE1	GLN	B	20	-7.843	1.105	-4.393	1.00	18.76
4299	NE2	GLN	B	20	-9.742	2.243	-4.794	1.00	25.21
4302	C	GLN	B	20	-5.913	4.671	-7.010	1.00	36.44
4303	O	GLN	B	20	-5.929	5.728	-6.386	1.00	37.25
4307	N	GLN	B	21	-6.149	4.624	-8.317	1.00	36.71
4309	CA	GLN	B	21	-6.707	5.800	-8.986	1.00	36.79
4311	CB	GLN	B	21	-5.705	6.439	-9.962	1.00	37.03
4314	CG	GLN	B	21	-4.639	7.334	-9.262	1.00	37.91
4317	CD	GLN	B	21	-5.064	8.800	-9.068	1.00	38.95
4318	OE1	GLN	B	21	-6.116	9.233	-9.551	1.00	40.45
4319	NE2	GLN	B	21	-4.236	9.560	-8.355	1.00	39.76
4322	C	GLN	B	21	-8.040	5.450	-9.653	1.00	36.53
4323	O	GLN	B	21	-8.166	4.408	-10.313	1.00	36.40
4324	N	PRO	B	22	-9.047	6.304	-9.464	1.00	36.31
4325	CA	PRO	B	22	-10.382	6.008	-9.979	1.00	36.04
4327	CB	PRO	B	22	-11.271	7.093	-9.346	1.00	36.07
4330	CG	PRO	B	22	-10.423	7.815	-8.380	1.00	36.23
4333	CD	PRO	B	22	-9.005	7.615	-8.789	1.00	36.26
4336	C	PRO	B	22	-10.424	6.113	-11.494	1.00	35.90
4337	O	PRO	B	22	-9.489	6.637	-12.106	1.00	36.05
4338	N	LEU	B	23	-11.492	5.599	-12.089	1.00	35.54
4340	CA	LEU	B	23	-11.746	5.803	-13.504	1.00	35.33
4342	CB	LEU	B	23	-12.823	4.837	-13.998	1.00	35.28
4345	CG	LEU	B	23	-12.541	3.346	-13.789	1.00	35.36
4347	CD1	LEU	B	23	-13.675	2.517	-14.372	1.00	35.32
4351	CD2	LEU	B	23	-11.199	2.949	-14.403	1.00	35.65
4355	C	LEU	B	23	-12.202	7.247	-13.685	1.00	35.19
4356	O	LEU	B	23	-13.131	7.692	-13.008	1.00	35.21
4357	N	ASN	B	24	-11.529	7.978	-14.572	1.00	34.72
4359	CA	ASN	B	24	-11.889	9.357	-14.884	1.00	34.51
4361	CB	ASN	B	24	-10.658	10.134	-15.375	1.00	34.65
4364	CG	ASN	B	24	-10.893	11.639	-15.443	1.00	35.54

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
4365	OD1	ASN	B	24	-11.928	12.146	-15.004	1.00	37.54
4366	ND2	ASN	B	24	-9.920	12.360	-15.994	1.00	36.15
4369	C	ASN	B	24	-13.011	9.376	-15.920	1.00	33.84
4370	O	ASN	B	24	-12.798	9.658	-17.101	1.00	33.82
4371	N	GLU	B	25	-14.210	9.053	-15.454	1.00	32.91
4373	CA	GLU	B	25	-15.400	9.027	-16.294	1.00	32.15
4375	CB	GLU	B	25	-15.363	7.853	-17.287	1.00	32.64
4378	CG	GLU	B	25	-14.912	6.522	-16.697	1.00	33.98
4381	CD	GLU	B	25	-15.039	5.353	-17.665	1.00	36.09
4382	OE1	GLU	B	25	-14.328	4.344	-17.468	1.00	37.86
4383	OE2	GLU	B	25	-15.853	5.424	-18.614	1.00	38.09
4384	C	GLU	B	25	-16.637	8.943	-15.405	1.00	30.71
4385	O	GLU	B	25	-16.546	8.590	-14.225	1.00	30.59
4386	N	GLU	B	26	-17.786	9.295	-15.969	1.00	28.93
4388	CA	GLU	B	26	-19.037	9.228	-15.239	1.00	27.75
4390	CB	GLU	B	26	-20.111	10.094	-15.905	1.00	28.26
4393	CG	GLU	B	26	-21.115	10.688	-14.923	1.00	30.31
4396	CD	GLU	B	26	-21.800	11.930	-15.464	1.00	33.30
4397	OE1	GLU	B	26	-23.048	11.928	-15.556	1.00	34.92
4398	OE2	GLU	B	26	-21.090	12.905	-15.801	1.00	35.14
4399	C	GLU	B	26	-19.492	7.776	-15.181	1.00	25.74
4400	O	GLU	B	26	-19.273	7.004	-16.115	1.00	25.10
4401	N	PHE	B	27	-20.125	7.413	-14.075	1.00	23.65
4403	CA	PHE	B	27	-20.710	6.094	-13.949	1.00	22.47
4405	CB	PHE	B	27	-21.360	5.910	-12.580	1.00	21.78
4408	CG	PHE	B	27	-22.025	4.579	-12.420	1.00	20.51
4409	CD1	PHE	B	27	-21.272	3.454	-12.130	1.00	18.84
4411	CE1	PHE	B	27	-21.867	2.223	-12.003	1.00	18.82
4413	CZ	PHE	B	27	-23.242	2.095	-12.161	1.00	18.47
4415	CE2	PHE	B	27	-24.003	3.202	-12.459	1.00	19.59
4417	CD2	PHE	B	27	-23.400	4.440	-12.591	1.00	19.83
4419	C	PHE	B	27	-21.774	5.896	-15.017	1.00	22.16
4420	O	PHE	B	27	-22.550	6.809	-15.310	1.00	22.26
4421	N	ARG	B	28	-21.798	4.704	-15.596	1.00	21.83
4423	CA	ARG	B	28	-22.934	4.271	-16.397	1.00	22.27
4425	CB	ARG	B	28	-22.643	4.362	-17.898	1.00	22.85
4428	CG	ARG	B	28	-21.399	3.644	-18.368	1.00	25.70
4431	CD	ARG	B	28	-20.797	4.201	-19.666	1.00	29.30
4434	NE	ARG	B	28	-19.436	3.695	-19.846	1.00	32.02
4436	CZ	ARG	B	28	-19.125	2.505	-20.363	1.00	34.35
4437	NH1	ARG	B	28	-20.072	1.673	-20.793	1.00	35.52
4440	NH2	ARG	B	28	-17.848	2.144	-20.459	1.00	35.35
4443	C	ARG	B	28	-23.286	2.849	-15.994	1.00	21.49
4444	O	ARG	B	28	-22.394	2.047	-15.725	1.00	20.35
4445	N	PRO	B	29	-24.577	2.530	-15.924	1.00	21.49
4446	CA	PRO	B	29	-25.000	1.189	-15.491	1.00	21.35
4448	CB	PRO	B	29	-26.533	1.242	-15.563	1.00	21.45
4451	CG	PRO	B	29	-26.878	2.477	-16.305	1.00	22.07
4454	CD	PRO	B	29	-25.721	3.415	-16.213	1.00	21.83



# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
4457	C	PRO	B	29	-24.432	0.039	-16.334	1.00	20.88
4458	O	PRO	B	29	-24.280	-1.057	-15.804	1.00	20.83
4459	N	GLU	B	30	-24.076	0.289	-17.593	1.00	20.54
4461	CA	GLU	B	30	-23.489	-0.753	-18.439	1.00	20.88
4463	CB	GLU	B	30	-23.369	-0.290	-19.891	1.00	21.30
4466	CG	GLU	B	30	-24.670	0.226	-20.480	1.00	24.00
4469	CD	GLU	B	30	-24.699	1.741	-20.540	1.00	27.46
4470	OE1	GLU	B	30	-25.159	2.369	-19.560	1.00	27.28
4471	OE2	GLU	B	30	-24.234	2.303	-21.562	1.00	30.43
4472	C	GLU	B	30	-22.126	-1.226	-17.937	1.00	19.67
4473	O	GLU	B	30	-21.675	-2.297	-18.310	1.00	19.61
4474	N	MET	B	31	-21.475	-0.425	-17.092	1.00	19.18
4476	CA	MET	B	31	-20.247	-0.840	-16.408	1.00	18.72
4478	CB	MET	B	31	-19.775	0.251	-15.451	1.00	18.80
4481	CG	MET	B	31	-19.242	1.484	-16.145	1.00	19.60
4484	SD	MET	B	31	-18.784	2.784	-14.992	1.00	19.64
4485	CE	MET	B	31	-17.796	3.811	-16.068	1.00	20.33
4489	C	MET	B	31	-20.405	-2.143	-15.608	1.00	17.99
4490	O	MET	B	31	-19.422	-2.834	-15.360	1.00	18.01
4491	N	LEU	B	32	-21.629	-2.463	-15.191	1.00	17.19
4493	CA	LEU	B	32	-21.883	-3.684	-14.419	1.00	16.71
4495	CB	LEU	B	32	-22.773	-3.383	-13.205	1.00	17.00
4498	CG	LEU	B	32	-22.084	-2.882	-11.928	1.00	18.30
4500	CD1	LEU	B	32	-21.044	-3.883	-11.441	1.00	18.08
4504	CD2	LEU	B	32	-21.464	-1.517	-12.159	1.00	18.86
4508	C	LEU	B	32	-22.512	-4.814	-15.240	1.00	16.13
4509	O	LEU	B	32	-22.620	-5.934	-14.756	1.00	14.69
4510	N	GLN	B	33	-22.926	-4.528	-16.469	1.00	15.72
4512	CA	GLN	B	33	-23.521	-5.551	-17.332	1.00	16.16
4514	CB	GLN	B	33	-23.896	-4.951	-18.685	1.00	16.69
4517	CG	GLN	B	33	-24.773	-5.824	-19.541	1.00	18.87
4520	CD	GLN	B	33	-25.350	-5.052	-20.707	1.00	22.92
4521	OE1	GLN	B	33	-26.393	-4.410	-20.575	1.00	27.06
4522	NE2	GLN	B	33	-24.666	-5.094	-21.843	1.00	25.66
4525	C	GLN	B	33	-22.567	-6.722	-17.542	1.00	15.74
4526	O	GLN	B	33	-21.430	-6.533	-17.980	1.00	16.35
4527	N	GLY	B	34	-23.023	-7.926	-17.209	1.00	14.59
4529	CA	GLY	B	34	-22.210	-9.122	-17.354	1.00	14.57
4532	C	GLY	B	34	-21.118	-9.320	-16.309	1.00	14.56
4533	O	GLY	B	34	-20.411	-10.330	-16.341	1.00	15.11
4534	N	LYS	B	35	-20.965	-8.374	-15.385	1.00	13.95
4536	CA	LYS	B	35	-19.950	-8.486	-14.346	1.00	14.32
4538	CB	LYS	B	35	-19.647	-7.130	-13.703	1.00	14.03
4541	CG	LYS	B	35	-19.049	-6.106	-14.674	1.00	16.08
4544	CD	LYS	B	35	-17.652	-6.486	-15.139	1.00	18.35
4547	CE	LYS	B	35	-17.178	-5.575	-16.275	1.00	20.67
4550	NZ	LYS	B	35	-15.715	-5.720	-16.509	1.00	22.25
4554	C	LYS	B	35	-20.388	-9.486	-13.303	1.00	14.06
4555	O	LYS	B	35	-21.572	-9.706	-13.108	1.00	14.30

## FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
4556	N	LYS	B	36	-19.411	-10.112	-12.662	1.00	13.32
4558	CA	LYS	B	36	-19.635	-11.213	-11.743	1.00	13.15
4560	CB	LYS	B	36	-18.679	-12.364	-12.075	1.00	13.62
4563	CG	LYS	B	36	-18.984	-12.986	-13.432	1.00	15.14
4566	CD	LYS	B	36	-17.868	-13.860	-13.973	1.00	18.88
4569	CE	LYS	B	36	-18.182	-14.205	-15.429	1.00	20.40
4572	NZ	LYS	B	36	-17.391	-15.346	-15.955	1.00	21.94
4576	C	LYS	B	36	-19.431	-10.707	-10.320	1.00	12.69
4577	O	LYS	B	36	-18.317	-10.362	-9.937	1.00	12.18
4578	N	VAL	B	37	-20.512	-10.651	-9.539	1.00	11.50
4580	CA	VAL	B	37	-20.479	-9.945	-8.266	1.00	11.19
4582	CB	VAL	B	37	-21.275	-8.617	-8.352	1.00	10.89
4584	CG1	VAL	B	37	-21.053	-7.772	-7.100	1.00	11.91
4588	CG2	VAL	B	37	-20.882	-7.853	-9.627	1.00	11.17
4592	C	VAL	B	37	-21.003	-10.788	-7.118	1.00	11.28
4593	O	VAL	B	37	-22.047	-11.420	-7.238	1.00	11.91
4594	N	ILE	B	38	-20.245	-10.811	-6.025	1.00	11.11
4596	CA	ILE	B	38	-20.697	-11.350	-4.743	1.00	11.28
4598	CB	ILE	B	38	-19.535	-12.065	-4.019	1.00	11.56
4600	CG1	ILE	B	38	-19.256	-13.419	-4.672	1.00	12.32
4603	CD1	ILE	B	38	-17.990	-14.080	-4.186	1.00	12.03
4607	CG2	ILE	B	38	-19.795	-12.190	-2.502	1.00	11.25
4611	C	ILE	B	38	-21.200	-10.192	-3.890	1.00	11.21
4612	O	ILE	B	38	-20.535	-9.157	-3.788	1.00	10.09
4613	N	VAL	B	39	-22.340	-10.386	-3.232	1.00	10.84
4615	CA	VAL	B	39	-22.801	-9.463	-2.205	1.00	11.17
4617	CB	VAL	B	39	-24.083	-8.692	-2.609	1.00	11.06
4619	CG1	VAL	B	39	-24.330	-7.544	-1.633	1.00	11.93
4623	CG2	VAL	B	39	-23.991	-8.167	-4.041	1.00	12.80
4627	C	VAL	B	39	-23.086	-10.263	-0.948	1.00	10.67
4628	O	VAL	B	39	-23.924	-11.165	-0.961	1.00	10.68
4629	N	THR	B	40	-22.377	-9.959	0.132	1.00	10.45
4631	CA	THR	B	40	-22.686	-10.569	1.416	1.00	10.33
4633	CB	THR	B	40	-21.437	-10.870	2.246	1.00	10.35
4635	OG1	THR	B	40	-20.872	-9.645	2.756	1.00	11.62
4637	CG2	THR	B	40	-20.321	-11.525	1.419	1.00	10.86
4641	C	THR	B	40	-23.661	-9.713	2.211	1.00	10.47
4642	O	THR	B	40	-23.885	-8.546	1.918	1.00	11.01
4643	N	GLY	B	41	-24.269	-10.331	3.212	1.00	10.59
4645	CA	GLY	B	41	-25.315	-9.686	3.980	1.00	10.74
4648	C	GLY	B	41	-26.423	-9.163	3.092	1.00	11.18
4649	O	GLY	B	41	-26.892	-8.039	3.266	1.00	10.32
4650	N	ALA	B	42	-26.859	-9.992	2.138	1.00	11.14
4652	CA	ALA	B	42	-27.712	-9.499	1.054	1.00	10.96
4654	CB	ALA	B	42	-27.064	-9.819	-0.287	1.00	11.72
4658	C	ALA	B	42	-29.164	-9.972	1.094	1.00	11.56
4659	O	ALA	B	42	-29.892	-9.834	0.106	1.00	12.32
4660	N	SER	B	43	-29.599	-10.461	2.247	1.00	11.19
4662	CA	SER	B	43	-30.968	-10.948	2.405	1.00	11.28

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
4664	CB	SER	B	43	-31.034	-12.021	3.492	1.00	11.43
4667	OG	SER	B	43	-30.663	-11.501	4.763	1.00	11.82
4669	C	SER	B	43	-31.921	-9.823	2.751	1.00	10.78
4670	O	SER	B	43	-33.129	-9.955	2.603	1.00	10.88
4671	N	LYS	B	44	-31.365	-8.714	3.237	1.00	10.94
4673	CA	LYS	B	44	-32.156	-7.551	3.606	1.00	10.46
4675	CB	LYS	B	44	-32.811	-7.742	4.970	1.00	11.62
4678	CG	LYS	B	44	-31.868	-8.011	6.083	1.00	12.64
4681	CD	LYS	B	44	-32.632	-8.418	7.348	1.00	15.79
4684	CE	LYS	B	44	-31.707	-8.666	8.530	1.00	17.74
4687	NZ	LYS	B	44	-32.515	-8.929	9.774	1.00	18.83
4691	C	LYS	B	44	-31.278	-6.304	3.603	1.00	10.34
4692	O	LYS	B	44	-30.098	-6.365	3.266	1.00	10.13
4693	N	GLY	B	45	-31.872	-5.170	3.956	1.00	10.24
4695	CA	GLY	B	45	-31.121	-3.936	4.129	1.00	9.78
4698	C	GLY	B	45	-30.421	-3.471	2.864	1.00	9.92
4699	O	GLY	B	45	-30.920	-3.642	1.766	1.00	9.73
4700	N	ILE	B	46	-29.260	-2.847	3.051	1.00	9.83
4702	CA	ILE	B	46	-28.482	-2.284	1.967	1.00	10.71
4704	CB	ILE	B	46	-27.310	-1.427	2.560	1.00	10.90
4706	CG1	ILE	B	46	-27.860	-0.274	3.417	1.00	11.85
4709	CD1	ILE	B	46	-26.916	0.187	4.490	1.00	12.01
4713	CG2	ILE	B	46	-26.430	-0.898	1.460	1.00	11.89
4717	C	ILE	B	46	-27.977	-3.367	1.008	1.00	10.36
4718	O	ILE	B	46	-27.950	-3.158	-0.198	1.00	10.94
4719	N	GLY	B	47	-27.585	-4.522	1.547	1.00	10.39
4721	CA	GLY	B	47	-27.108	-5.631	0.737	1.00	10.40
4724	C	GLY	B	47	-28.163	-6.101	-0.252	1.00	10.58
4725	O	GLY	B	47	-27.870	-6.321	-1.422	1.00	10.10
4726	N	ARG	B	48	-29.390	-6.268	0.215	1.00	10.36
4728	CA	ARG	B	48	-30.495	-6.643	-0.669	1.00	10.85
4730	CB	ARG	B	48	-31.804	-6.838	0.116	1.00	10.81
4733	CG	ARG	B	48	-33.065	-6.998	-0.755	1.00	12.26
4736	CD	ARG	B	48	-34.283	-7.475	0.020	1.00	13.95
4739	NE	ARG	B	48	-34.603	-6.543	1.096	1.00	15.81
4741	CZ	ARG	B	48	-35.534	-6.735	2.029	1.00	18.10
4742	NH1	ARG	B	48	-36.298	-7.823	2.020	1.00	18.81
4745	NH2	ARG	B	48	-35.720	-5.820	2.971	1.00	18.46
4748	C	ARG	B	48	-30.680	-5.594	-1.767	1.00	10.59
4749	O	ARG	B	48	-30.843	-5.937	-2.929	1.00	10.42
4750	N	GLU	B	49	-30.627	-4.313	-1.410	1.00	10.73
4752	CA	GLU	B	49	-30.780	-3.266	-2.417	1.00	10.56
4754	CB	GLU	B	49	-30.895	-1.889	-1.775	1.00	11.33
4757	CG	GLU	B	49	-32.095	-1.721	-0.847	1.00	11.49
4760	CD	GLU	B	49	-33.433	-2.050	-1.499	1.00	16.05
4761	OE1	GLU	B	49	-34.297	-2.645	-0.814	1.00	16.08
4762	OE2	GLU	B	49	-33.633	-1.713	-2.694	1.00	18.16
4763	C	GLU	B	49	-29.634	-3.275	-3.414	1.00	10.64
4764	O	GLU	B	49	-29.848	-3.010	-4.588	1.00	11.13

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
4765	N	MET	B	50	-28.428	-3.585	-2.958	1.00	10.44
4767	CA	MET	B	50	-27.299	-3.700	-3.876	1.00	10.75
4769	CB	MET	B	50	-25.982	-3.888	-3.118	1.00	10.94
4772	CG	MET	B	50	-25.500	-2.599	-2.496	1.00	11.45
4775	SD	MET	B	50	-23.833	-2.637	-1.809	1.00	12.29
4776	CE	MET	B	50	-24.061	-3.638	-0.349	1.00	11.44
4780	C	MET	B	50	-27.528	-4.833	-4.877	1.00	11.28
4781	O	MET	B	50	-27.306	-4.658	-6.072	1.00	11.30
4782	N	ALA	B	51	-27.994	-5.980	-4.401	1.00	11.40
4784	CA	ALA	B	51	-28.326	-7.096	-5.284	1.00	11.74
4786	CB	ALA	B	51	-28.836	-8.277	-4.479	1.00	11.64
4790	C	ALA	B	51	-29.352	-6.677	-6.334	1.00	11.49
4791	O	ALA	B	51	-29.209	-6.998	-7.507	1.00	11.83
4792	N	TYR	B	52	-30.366	-5.927	-5.923	1.00	11.06
4794	CA	TYR	B	52	-31.413	-5.496	-6.840	1.00	11.42
4796	CB	TYR	B	52	-32.560	-4.833	-6.078	1.00	11.42
4799	CG	TYR	B	52	-33.399	-5.774	-5.236	1.00	12.30
4800	CD1	TYR	B	52	-33.282	-7.162	-5.342	1.00	12.93
4802	CE1	TYR	B	52	-34.069	-8.006	-4.560	1.00	13.87
4804	CZ	TYR	B	52	-34.975	-7.467	-3.676	1.00	14.55
4805	OH	TYR	B	52	-35.756	-8.313	-2.908	1.00	17.23
4807	CE2	TYR	B	52	-35.101	-6.110	-3.548	1.00	14.56
4809	CD2	TYR	B	52	-34.314	-5.266	-4.327	1.00	14.92
4811	C	TYR	B	52	-30.883	-4.549	-7.905	1.00	11.61
4812	O	TYR	B	52	-31.247	-4.680	-9.066	1.00	12.01
4813	N	HIS	B	53	-30.021	-3.600	-7.528	1.00	11.20
4815	CA	HIS	B	53	-29.437	-2.693	-8.515	1.00	11.41
4817	CB	HIS	B	53	-28.589	-1.621	-7.839	1.00	11.43
4820	CG	HIS	B	53	-29.379	-0.476	-7.303	1.00	11.70
4821	ND1	HIS	B	53	-30.181	0.313	-8.098	1.00	14.86
4823	CE1	HIS	B	53	-30.743	1.248	-7.354	1.00	14.75
4825	NE2	HIS	B	53	-30.341	1.087	-6.109	1.00	13.92
4827	CD2	HIS	B	53	-29.480	0.024	-6.050	1.00	13.65
4829	C	HIS	B	53	-28.560	-3.451	-9.497	1.00	11.22
4830	O	HIS	B	53	-28.610	-3.200	-10.695	1.00	12.07
4831	N	LEU	B	54	-27.754	-4.372	-8.980	1.00	11.26
4833	CA	LEU	B	54	-26.889	-5.180	-9.823	1.00	11.80
4835	CB	LEU	B	54	-26.003	-6.090	-8.977	1.00	11.35
4838	CG	LEU	B	54	-24.920	-5.357	-8.182	1.00	11.68
4840	CD1	LEU	B	54	-24.424	-6.229	-7.039	1.00	11.98
4844	CD2	LEU	B	54	-23.764	-4.906	-9.092	1.00	12.69
4848	C	LEU	B	54	-27.722	-5.983	-10.816	1.00	11.95
4849	O	LEU	B	54	-27.373	-6.073	-11.991	1.00	12.30
4850	N	ALA	B	55	-28.835	-6.540	-10.348	1.00	12.23
4852	CA	ALA	B	55	-29.738	-7.299	-11.204	1.00	12.51
4854	CB	ALA	B	55	-30.878	-7.867	-10.382	1.00	12.61
4858	C	ALA	B	55	-30.282	-6.429	-12.343	1.00	13.29
4859	O	ALA	B	55	-30.268	-6.825	-13.511	1.00	12.82
4860	N	LYS	B	56	-30.753	-5.240	-12.000	1.00	13.47

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
4862	CA	LYS	B	56	-31.265	-4.302	-12.997	1.00	14.78
4864	CB	LYS	B	56	-31.794	-3.045	-12.320	1.00	15.21
4867	CG	LYS	B	56	-33.150	-3.214	-11.665	1.00	18.77
4870	CD	LYS	B	56	-33.802	-1.864	-11.341	1.00	21.92
4873	CE	LYS	B	56	-33.504	-1.411	-9.912	1.00	24.95
4876	NZ	LYS	B	56	-34.617	-0.581	-9.354	1.00	25.95
4880	C	LYS	B	56	-30.202	-3.930	-14.046	1.00	14.64
4881	O	LYS	B	56	-30.541	-3.667	-15.203	1.00	15.61
4882	N	MET	B	57	-28.930	-3.924	-13.640	1.00	14.23
4884	CA	MET	B	57	-27.812	-3.617	-14.529	1.00	14.34
4886	CB	MET	B	57	-26.634	-3.084	-13.710	1.00	14.23
4889	CG	MET	B	57	-26.908	-1.759	-13.031	1.00	16.36
4892	SD	MET	B	57	-25.547	-1.291	-11.913	1.00	21.40
4893	CE	MET	B	57	-26.338	-0.108	-10.855	1.00	20.93
4897	C	MET	B	57	-27.358	-4.826	-15.359	1.00	13.43
4898	O	MET	B	57	-26.489	-4.704	-16.224	1.00	13.77
4899	N	GLY	B	58	-27.929	-5.995	-15.092	1.00	12.87
4901	CA	GLY	B	58	-27.622	-7.198	-15.840	1.00	12.60
4904	C	GLY	B	58	-26.355	-7.904	-15.412	1.00	12.64
4905	O	GLY	B	58	-25.724	-8.601	-16.222	1.00	12.60
4906	N	ALA	B	59	-25.976	-7.729	-14.149	1.00	12.67
4908	CA	ALA	B	59	-24.853	-8.450	-13.579	1.00	12.49
4910	CB	ALA	B	59	-24.352	-7.744	-12.318	1.00	13.04
4914	C	ALA	B	59	-25.215	-9.892	-13.249	1.00	13.02
4915	O	ALA	B	59	-26.388	-10.239	-13.127	1.00	12.97
4916	N	HIS	B	60	-24.194	-10.731	-13.122	1.00	12.99
4918	CA	HIS	B	60	-24.330	-12.015	-12.441	1.00	13.22
4920	CB	HIS	B	60	-23.277	-13.007	-12.914	1.00	13.72
4923	CG	HIS	B	60	-23.336	-13.325	-14.374	1.00	13.97
4924	ND1	HIS	B	60	-24.021	-14.413	-14.867	1.00	14.72
4926	CE1	HIS	B	60	-23.862	-14.472	-16.178	1.00	16.58
4928	NE2	HIS	B	60	-23.095	-13.462	-16.553	1.00	15.42
4930	CD2	HIS	B	60	-22.748	-12.733	-15.441	1.00	14.82
4932	C	HIS	B	60	-24.122	-11.754	-10.962	1.00	13.22
4933	O	HIS	B	60	-23.175	-11.064	-10.592	1.00	12.64
4934	N	VAL	B	61	-24.978	-12.313	-10.114	1.00	13.18
4936	CA	VAL	B	61	-24.894	-12.069	-8.674	1.00	13.14
4938	CB	BVAL	B	61	-25.986	-11.093	-8.136	0.35	12.98
4939	CB	AVAL	B	61	-26.028	-11.118	-8.199	0.65	13.49
4942	CG1BVAL	B	61	-25.700	-9.668	-8.572	0.35	12.81	
4943	CG1AVAL	B	61	-25.784	-10.644	-6.786	0.65	14.74	
4950	CG2BVAL	B	61	-27.397	-11.534	-8.549	0.35	12.59	
4951	CG2AVAL	B	61	-26.188	-9.941	-9.155	0.65	13.97	
4958	C	VAL	B	61	-24.974	-13.364	-7.891	1.00	12.92
4959	O	VAL	B	61	-25.766	-14.252	-8.213	1.00	12.38
4960	N	VAL	B	62	-24.145	-13.466	-6.861	1.00	12.25
4962	CA	VAL	B	62	-24.303	-14.499	-5.857	1.00	12.23
4964	CB	VAL	B	62	-23.119	-15.481	-5.824	1.00	12.33
4966	CG1	VAL	B	62	-23.301	-16.504	-4.717	1.00	13.22

## FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
4970	CG2	VAL	B	62	-22.962	-16.171	-7.181	1.00	13.64
4974	C	VAL	B	62	-24.452	-13.776	-4.530	1.00	12.12
4975	O	VAL	B	62	-23.599	-12.970	-4.155	1.00	12.10
4976	N	VAL	B	63	-25.548	-14.054	-3.837	1.00	11.41
4978	CA	VAL	B	63	-25.850	-13.434	-2.559	1.00	11.23
4980	CB	VAL	B	63	-27.268	-12.801	-2.536	1.00	11.45
4982	CG1	VAL	B	63	-28.369	-13.810	-2.845	1.00	12.29
4986	CG2	VAL	B	63	-27.341	-11.610	-3.490	1.00	12.95
4990	C	VAL	B	63	-25.716	-14.428	-1.421	1.00	11.27
4991	O	VAL	B	63	-25.950	-15.624	-1.599	1.00	11.43
4992	N	THR	B	64	-25.345	-13.928	-0.251	1.00	11.16
4994	CA	THR	B	64	-25.289	-14.742	0.941	1.00	10.94
4996	CB	THR	B	64	-23.881	-15.367	1.092	1.00	11.01
4998	OG1	THR	B	64	-23.873	-16.336	2.151	1.00	11.55
5000	CG2	THR	B	64	-22.810	-14.327	1.455	1.00	10.73
5004	C	THR	B	64	-25.743	-14.004	2.202	1.00	11.00
5005	O	THR	B	64	-25.799	-12.767	2.240	1.00	10.83
5006	N	ALA	B	65	-26.082	-14.821	3.188	1.00	10.69
5008	CA	ALA	B	65	-26.584	-14.488	4.527	1.00	10.22
5010	CB	ALA	B	65	-27.824	-13.624	4.480	1.00	10.27
5014	C	ALA	B	65	-26.890	-15.844	5.171	1.00	10.61
5015	O	ALA	B	65	-26.720	-16.885	4.541	1.00	10.78
5016	N	ARG	B	66	-27.373	-15.862	6.407	1.00	11.87
5018	CA	ARG	B	66	-27.688	-17.139	7.050	1.00	12.24
5020	CB	ARG	B	66	-27.682	-17.001	8.573	1.00	11.88
5023	CG	ARG	B	66	-26.308	-16.697	9.161	1.00	10.67
5026	CD	ARG	B	66	-26.333	-16.321	10.626	1.00	10.36
5029	NE	ARG	B	66	-27.156	-15.139	10.856	1.00	11.69
5031	CZ	ARG	B	66	-27.501	-14.685	12.049	1.00	13.13
5032	NH1	ARG	B	66	-28.268	-13.612	12.149	1.00	14.08
5035	NH2	ARG	B	66	-27.085	-15.292	13.150	1.00	16.68
5038	C	ARG	B	66	-29.026	-17.729	6.590	1.00	13.55
5039	O	ARG	B	66	-29.167	-18.958	6.519	1.00	14.49
5040	N	SER	B	67	-29.994	-16.868	6.278	1.00	14.61
5042	CA	SER	B	67	-31.380	-17.315	6.057	1.00	15.17
5044	CB	BSER	B	67	-32.348	-16.251	6.568	0.35	15.27
5045	CB	ASER	B	67	-32.378	-16.274	6.552	0.65	15.48
5050	OG	BSER	B	67	-31.936	-15.747	7.829	0.35	15.23
5051	OG	ASER	B	67	-33.718	-16.653	6.243	0.65	16.23
5054	C	SER	B	67	-31.676	-17.641	4.596	1.00	15.57
5055	O	SER	B	67	-31.746	-16.751	3.757	1.00	15.08
5056	N	LYS	B	68	-31.879	-18.921	4.306	1.00	16.31
5058	CA	LYS	B	68	-32.209	-19.356	2.948	1.00	16.94
5060	CB	LYS	B	68	-32.230	-20.887	2.853	1.00	17.69
5063	CG	LYS	B	68	-33.262	-21.557	3.738	1.00	20.27
5066	CD	LYS	B	68	-33.168	-23.071	3.671	1.00	23.39
5069	CE	LYS	B	68	-34.158	-23.700	4.631	1.00	25.32
5072	NZ	LYS	B	68	-35.566	-23.319	4.295	1.00	26.88
5076	C	LYS	B	68	-33.544	-18.766	2.482	1.00	17.00

## FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
5077	O	LYS	B	68	-33.697	-18.424	1.321	1.00	16.21
5078	N	GLU	B	69	-34.506	-18.646	3.394	1.00	17.16
5080	CA	GLU	B	69	-35.846	-18.171	3.036	1.00	18.03
5082	CB	GLU	B	69	-36.781	-18.309	4.246	1.00	19.01
5085	CG	GLU	B	69	-38.074	-17.512	4.186	1.00	22.91
5088	CD	GLU	B	69	-38.962	-17.761	5.395	1.00	27.61
5089	OE1	GLU	B	69	-38.646	-18.679	6.180	1.00	29.79
5090	OE2	GLU	B	69	-39.970	-17.032	5.562	1.00	31.63
5091	C	GLU	B	69	-35.831	-16.738	2.491	1.00	16.82
5092	O	GLU	B	69	-36.443	-16.448	1.464	1.00	16.76
5093	N	THR	B	70	-35.110	-15.851	3.170	1.00	15.59
5095	CA	THR	B	70	-35.016	-14.462	2.743	1.00	14.70
5097	CB	THR	B	70	-34.575	-13.560	3.920	1.00	15.40
5099	OG1	THR	B	70	-33.385	-14.074	4.513	1.00	15.62
5101	CG2	THR	B	70	-35.596	-13.629	5.048	1.00	16.12
5105	C	THR	B	70	-34.088	-14.317	1.536	1.00	13.87
5106	O	THR	B	70	-34.341	-13.493	0.665	1.00	13.80
5107	N	LEU	B	71	-33.018	-15.106	1.483	1.00	12.53
5109	CA	LEU	B	71	-32.147	-15.108	0.303	1.00	12.28
5111	CB	LEU	B	71	-30.931	-16.017	0.507	1.00	12.21
5114	CG	LEU	B	71	-29.894	-15.505	1.494	1.00	12.18
5116	CD1	LEU	B	71	-28.896	-16.600	1.831	1.00	12.74
5120	CD2	LEU	B	71	-29.176	-14.298	0.915	1.00	13.61
5124	C	LEU	B	71	-32.906	-15.541	-0.946	1.00	12.33
5125	O	LEU	B	71	-32.691	-14.998	-2.024	1.00	11.70
5126	N	GLN	B	72	-33.799	-16.513	-0.788	1.00	12.93
5128	CA	GLN	B	72	-34.564	-17.053	-1.915	1.00	13.12
5130	CB	BGLN	B	72	-35.428	-18.239	-1.487	0.35	13.30
5131	CB	AGLN	B	72	-35.443	-18.234	-1.462	0.65	13.85
5136	CG	BGLN	B	72	-36.414	-18.681	-2.560	0.35	13.02
5137	CG	AGLN	B	72	-34.684	-19.551	-1.322	0.65	15.06
5142	CD	BGLN	B	72	-36.784	-20.145	-2.467	0.35	14.03
5143	CD	AGLN	B	72	-35.483	-20.691	-0.665	0.65	17.70
5144	OE1	BGLN	B	72	-36.967	-20.681	-1.371	0.35	15.69
5145	OE1	AGLN	B	72	-36.410	-20.467	0.127	0.65	19.97
5146	NE2	BGLN	B	72	-36.896	-20.796	-3.617	0.35	12.09
5147	NE2	AGLN	B	72	-35.100	-21.918	-0.985	0.65	20.50
5152	C	GLN	B	72	-35.434	-15.955	-2.527	1.00	13.02
5153	O	GLN	B	72	-35.541	-15.830	-3.752	1.00	12.87
5154	N	LYS	B	73	-36.032	-15.142	-1.671	1.00	12.47
5156	CA	LYS	B	73	-36.858	-14.031	-2.126	1.00	13.29
5158	CB	LYS	B	73	-37.586	-13.385	-0.944	1.00	14.34
5161	CG	LYS	B	73	-38.643	-14.289	-0.330	1.00	17.96
5164	CD	LYS	B	73	-39.199	-13.727	0.985	1.00	22.72
5167	CE	LYS	B	73	-40.199	-14.683	1.628	1.00	24.89
5170	NZ	LYS	B	73	-41.579	-14.514	1.087	1.00	27.34
5174	C	LYS	B	73	-36.037	-13.007	-2.894	1.00	12.55
5175	O	LYS	B	73	-36.473	-12.498	-3.930	1.00	12.96
5176	N	VAL	B	74	-34.828	-12.733	-2.411	1.00	12.04

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
5178	CA	VAL	B	74	-33.949	-11.792	-3.096	1.00	11.38
5180	CB	VAL	B	74	-32.681	-11.462	-2.263	1.00	11.18
5182	CG1	VAL	B	74	-31.667	-10.639	-3.067	1.00	10.96
5186	CG2	VAL	B	74	-33.089	-10.700	-1.012	1.00	12.21
5190	C	VAL	B	74	-33.597	-12.332	-4.480	1.00	11.57
5191	O	VAL	B	74	-33.693	-11.606	-5.459	1.00	11.53
5192	N	VAL	B	75	-33.243	-13.610	-4.561	1.00	11.67
5194	CA	VAL	B	75	-32.883	-14.209	-5.848	1.00	12.29
5196	CB	VAL	B	75	-32.376	-15.647	-5.695	1.00	12.69
5198	CG1	VAL	B	75	-31.018	-15.665	-5.005	1.00	12.85
5202	CG2	VAL	B	75	-32.297	-16.350	-7.052	1.00	13.10
5206	C	VAL	B	75	-34.068	-14.131	-6.813	1.00	12.56
5207	O	VAL	B	75	-33.894	-13.792	-7.989	1.00	12.16
5208	N	SER	B	76	-35.274	-14.413	-6.319	1.00	12.75
5210	CA	SER	B	76	-36.467	-14.358	-7.177	1.00	13.14
5212	CB	SER	B	76	-37.723	-14.746	-6.397	1.00	13.73
5215	OG	SER	B	76	-37.693	-16.123	-6.099	1.00	15.89
5217	C	SER	B	76	-36.650	-12.986	-7.803	1.00	13.16
5218	O	SER	B	76	-36.930	-12.873	-9.003	1.00	12.89
5219	N	HIS	B	77	-36.469	-11.939	-7.002	1.00	12.59
5221	CA	HIS	B	77	-36.637	-10.578	-7.493	1.00	13.20
5223	CB	HIS	B	77	-36.757	-9.581	-6.333	1.00	13.55
5226	CG	HIS	B	77	-37.289	-8.239	-6.740	1.00	17.44
5227	ND1	HIS	B	77	-38.485	-8.080	-7.409	1.00	21.59
5229	CE1	HIS	B	77	-38.690	-6.795	-7.642	1.00	22.70
5231	NE2	HIS	B	77	-37.679	-6.112	-7.136	1.00	21.19
5233	CD2	HIS	B	77	-36.788	-6.991	-6.571	1.00	21.20
5235	C	HIS	B	77	-35.498	-10.197	-8.436	1.00	12.76
5236	O	HIS	B	77	-35.735	-9.549	-9.448	1.00	12.83
5237	N	CYS	B	78	-34.275	-10.618	-8.123	1.00	12.54
5239	CA	CYS	B	78	-33.136	-10.370	-9.011	1.00	12.18
5241	CB	CYS	B	78	-31.841	-10.939	-8.418	1.00	11.72
5244	SG	CYS	B	78	-31.144	-10.004	-7.018	1.00	12.23
5245	C	CYS	B	78	-33.352	-10.976	-10.402	1.00	12.35
5246	O	CYS	B	78	-33.025	-10.360	-11.404	1.00	12.28
5247	N	LEU	B	79	-33.887	-12.192	-10.458	1.00	12.57
5249	CA	LEU	B	79	-34.106	-12.868	-11.732	1.00	12.97
5251	CB	LEU	B	79	-34.547	-14.317	-11.504	1.00	12.73
5254	CG	LEU	B	79	-33.460	-15.222	-10.909	1.00	12.61
5256	CD1	LEU	B	79	-32.236	-15.360	-11.821	1.00	12.90
5260	CD2	LEU	B	79	-34.040	-16.594	-10.574	1.00	12.64
5264	C	LEU	B	79	-35.142	-12.102	-12.544	1.00	13.48
5265	O	LEU	B	79	-34.977	-11.908	-13.742	1.00	14.04
5266	N	GLU	B	80	-36.180	-11.623	-11.867	1.00	14.29
5268	CA	GLU	B	80	-37.233	-10.859	-12.523	1.00	15.56
5270	CB	GLU	B	80	-38.426	-10.673	-11.589	1.00	16.58
5273	CG	GLU	B	80	-39.625	-10.069	-12.297	1.00	19.55
5276	CD	GLU	B	80	-40.962	-10.478	-11.716	1.00	22.06
5277	OE1	GLU	B	80	-41.016	-11.336	-10.799	1.00	22.99



## FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
5278	OE2	GLU	B	80	-41.968	-9.919	-12.193	1.00	25.64
5279	C	GLU	B	80	-36.732	-9.501	-13.023	1.00	15.11
5280	O	GLU	B	80	-37.161	-9.038	-14.084	1.00	14.85
5281	N	LEU	B	81	-35.808	-8.898	-12.276	1.00	14.72
5283	CA	LEU	B	81	-35.281	-7.570	-12.579	1.00	14.99
5285	CB	LEU	B	81	-34.556	-6.976	-11.369	1.00	15.34
5288	CG	LEU	B	81	-35.436	-6.452	-10.234	1.00	15.75
5290	CD1	LEU	B	81	-34.580	-6.181	-9.005	1.00	17.29
5294	CD2	LEU	B	81	-36.201	-5.208	-10.669	1.00	17.29
5298	C	LEU	B	81	-34.320	-7.586	-13.757	1.00	14.85
5299	O	LEU	B	81	-34.040	-6.527	-14.342	1.00	15.16
5300	N	GLY	B	82	-33.797	-8.762	-14.087	1.00	14.15
5302	CA	GLY	B	82	-32.937	-8.930	-15.249	1.00	14.12
5305	C	GLY	B	82	-31.481	-9.276	-14.993	1.00	14.28
5306	O	GLY	B	82	-30.624	-9.005	-15.837	1.00	14.31
5307	N	ALA	B	83	-31.184	-9.869	-13.837	1.00	13.95
5309	CA	ALA	B	83	-29.846	-10.376	-13.565	1.00	14.20
5311	CB	ALA	B	83	-29.814	-11.043	-12.204	1.00	14.07
5315	C	ALA	B	83	-29.460	-11.370	-14.657	1.00	14.38
5316	O	ALA	B	83	-30.309	-12.146	-15.104	1.00	13.64
5317	N	ALA	B	84	-28.211	-11.323	-15.130	1.00	14.52
5319	CA	ALA	B	84	-27.700	-12.346	-16.055	1.00	14.86
5321	CB	ALA	B	84	-26.265	-12.075	-16.409	1.00	14.96
5325	C	ALA	B	84	-27.836	-13.743	-15.451	1.00	14.79
5326	O	ALA	B	84	-28.164	-14.706	-16.143	1.00	15.68
5327	N	SER	B	85	-27.558	-13.832	-14.156	1.00	14.98
5329	CA	SER	B	85	-27.836	-15.012	-13.341	1.00	14.41
5331	CB	SER	B	85	-26.764	-16.091	-13.517	1.00	15.07
5334	OG	SER	B	85	-25.506	-15.693	-12.983	1.00	15.95
5336	C	SER	B	85	-27.899	-14.553	-11.889	1.00	14.07
5337	O	SER	B	85	-27.366	-13.505	-11.535	1.00	13.09
5338	N	ALA	B	86	-28.576	-15.318	-11.048	1.00	13.23
5340	CA	ALA	B	86	-28.638	-15.009	-9.627	1.00	13.31
5342	CB	ALA	B	86	-29.792	-14.073	-9.330	1.00	13.39
5346	C	ALA	B	86	-28.758	-16.295	-8.828	1.00	13.75
5347	O	ALA	B	86	-29.591	-17.150	-9.133	1.00	13.98
5348	N	HIS	B	87	-27.873	-16.451	-7.844	1.00	13.70
5350	CA	HIS	B	87	-27.847	-17.615	-6.973	1.00	13.32
5352	CB	HIS	B	87	-26.664	-18.525	-7.323	1.00	14.02
5355	CG	HIS	B	87	-26.683	-19.056	-8.722	1.00	16.44
5356	ND1	HIS	B	87	-27.212	-20.287	-9.048	1.00	20.96
5358	CE1	HIS	B	87	-27.062	-20.497	-10.345	1.00	20.56
5360	NE2	HIS	B	87	-26.422	-19.464	-10.864	1.00	21.18
5362	CD2	HIS	B	87	-26.167	-18.555	-9.867	1.00	18.86
5364	C	HIS	B	87	-27.672	-17.152	-5.539	1.00	13.09
5365	O	HIS	B	87	-27.132	-16.056	-5.289	1.00	11.68
5366	N	TYR	B	88	-28.090	-17.989	-4.597	1.00	12.65
5368	CA	TYR	B	88	-27.758	-17.786	-3.198	1.00	13.20
5370	CB	TYR	B	88	-29.010	-17.452	-2.385	1.00	13.05

## FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
5373	CG	TYR	B	88	-29.932	-18.627	-2.142	1.00	15.19
5374	CD1	TYR	B	88	-29.806	-19.405	-0.994	1.00	19.13
5376	CE1	TYR	B	88	-30.648	-20.481	-0.762	1.00	20.55
5378	CZ	TYR	B	88	-31.632	-20.776	-1.682	1.00	21.35
5379	OH	TYR	B	88	-32.483	-21.841	-1.455	1.00	25.30
5381	CE2	TYR	B	88	-31.780	-20.011	-2.830	1.00	20.23
5383	CD2	TYR	B	88	-30.931	-18.941	-3.049	1.00	18.92
5385	C	TYR	B	88	-27.059	-18.994	-2.592	1.00	13.17
5386	O	TYR	B	88	-27.248	-20.136	-3.030	1.00	13.72
5387	N	ILE	B	89	-26.259	-18.725	-1.569	1.00	13.13
5389	CA	ILE	B	89	-25.644	-19.747	-0.740	1.00	13.40
5391	CB	ILE	B	89	-24.164	-19.954	-1.114	1.00	13.47
5393	CG1	ILE	B	89	-24.003	-20.295	-2.599	1.00	14.51
5396	CD1	ILE	B	89	-22.569	-20.256	-3.077	1.00	16.49
5400	CG2	ILE	B	89	-23.535	-21.033	-0.237	1.00	14.36
5404	C	ILE	B	89	-25.774	-19.270	0.698	1.00	13.60
5405	O	ILE	B	89	-25.276	-18.203	1.042	1.00	13.98
5406	N	ALA	B	90	-26.434	-20.059	1.531	1.00	13.19
5408	CA	ALA	B	90	-26.672	-19.695	2.927	1.00	12.87
5410	CB	ALA	B	90	-28.039	-20.166	3.368	1.00	12.71
5414	C	ALA	B	90	-25.611	-20.254	3.858	1.00	12.96
5415	O	ALA	B	90	-25.173	-21.403	3.718	1.00	13.49
5416	N	GLY	B	91	-25.206	-19.430	4.822	1.00	12.42
5418	CA	GLY	B	91	-24.297	-19.860	5.861	1.00	11.92
5421	C	GLY	B	91	-23.919	-18.719	6.766	1.00	11.99
5422	O	GLY	B	91	-24.307	-17.572	6.528	1.00	11.49
5423	N	THR	B	92	-23.198	-19.035	7.833	1.00	11.98
5425	CA	THR	B	92	-22.797	-18.019	8.786	1.00	12.58
5427	CB	THR	B	92	-23.081	-18.430	10.238	1.00	12.35
5429	OG1	THR	B	92	-22.528	-17.430	11.104	1.00	12.85
5431	CG2	THR	B	92	-22.345	-19.723	10.629	1.00	13.17
5435	C	THR	B	92	-21.336	-17.659	8.616	1.00	12.55
5436	O	THR	B	92	-20.474	-18.537	8.479	1.00	13.03
5437	N	MET	B	93	-21.059	-16.364	8.647	1.00	12.38
5439	CA	MET	B	93	-19.698	-15.854	8.500	1.00	12.98
5441	CB	MET	B	93	-19.718	-14.435	7.915	1.00	12.86
5444	CG	MET	B	93	-20.148	-14.410	6.455	1.00	12.81
5447	SD	MET	B	93	-19.054	-15.248	5.320	1.00	13.60
5448	CE	MET	B	93	-19.954	-15.003	3.766	1.00	14.79
5452	C	MET	B	93	-18.934	-15.907	9.819	1.00	13.78
5453	O	MET	B	93	-17.817	-15.407	9.910	1.00	14.29
5454	N	GLU	B	94	-19.547	-16.499	10.844	1.00	14.48
5456	CA	GLU	B	94	-18.845	-16.902	12.060	1.00	15.20
5458	CB	GLU	B	94	-19.813	-17.381	13.133	1.00	15.81
5461	CG	GLU	B	94	-20.832	-16.384	13.627	1.00	17.81
5464	CD	GLU	B	94	-21.932	-17.095	14.383	1.00	21.28
5465	OE1	GLU	B	94	-22.884	-17.600	13.734	1.00	22.16
5466	OE2	GLU	B	94	-21.820	-17.194	15.627	1.00	24.40
5467	C	GLU	B	94	-17.916	-18.064	11.772	1.00	15.25

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
5468	O	GLU	B	94	-16.982	-18.305	12.529	1.00	15.57
5469	N	ASP	B	95	-18.205	-18.783	10.688	1.00	14.82
5471	CA	ASP	B	95	-17.494	-20.002	10.299	1.00	15.53
5473	CB	ASP	B	95	-18.518	-21.063	9.881	1.00	15.98
5476	CG	ASP	B	95	-17.896	-22.393	9.528	1.00	16.87
5477	OD1	ASP	B	95	-16.657	-22.469	9.399	1.00	18.17
5478	OD2	ASP	B	95	-18.582	-23.420	9.352	1.00	19.28
5479	C	ASP	B	95	-16.561	-19.648	9.160	1.00	15.28
5480	O	ASP	B	95	-16.995	-19.439	8.037	1.00	14.72
5481	N	MET	B	96	-15.267	-19.555	9.455	1.00	15.51
5483	CA	MET	B	96	-14.296	-19.126	8.459	1.00	15.54
5485	CB	MET	B	96	-12.930	-18.854	9.093	1.00	15.89
5488	CG	MET	B	96	-12.911	-17.797	10.179	1.00	16.96
5491	SD	MET	B	96	-13.574	-16.194	9.700	1.00	19.45
5492	CE	MET	B	96	-14.684	-15.854	11.010	1.00	19.14
5496	C	MET	B	96	-14.143	-20.150	7.342	1.00	15.09
5497	O	MET	B	96	-13.740	-19.798	6.238	1.00	14.82
5498	N	THR	B	97	-14.456	-21.413	7.628	1.00	15.60
5500	CA	THR	B	97	-14.465	-22.455	6.607	1.00	15.99
5502	CB	THR	B	97	-14.562	-23.845	7.253	1.00	16.62
5504	OG1	THR	B	97	-13.473	-24.014	8.170	1.00	18.56
5506	CG2	THR	B	97	-14.360	-24.934	6.218	1.00	17.61
5510	C	THR	B	97	-15.586	-22.239	5.594	1.00	15.64
5511	O	THR	B	97	-15.371	-22.379	4.388	1.00	15.56
5512	N	PHE	B	98	-16.769	-21.877	6.079	1.00	15.35
5514	CA	PHE	B	98	-17.846	-21.489	5.188	1.00	14.97
5516	CB	PHE	B	98	-19.134	-21.144	5.941	1.00	15.19
5519	CG	PHE	B	98	-20.178	-20.537	5.051	1.00	14.81
5520	CD1	PHE	B	98	-20.880	-21.335	4.156	1.00	15.21
5522	CE1	PHE	B	98	-21.824	-20.792	3.308	1.00	16.09
5524	CZ	PHE	B	98	-22.070	-19.426	3.331	1.00	16.70
5526	CE2	PHE	B	98	-21.371	-18.616	4.199	1.00	15.71
5528	CD2	PHE	B	98	-20.420	-19.167	5.055	1.00	15.07
5530	C	PHE	B	98	-17.433	-20.296	4.338	1.00	14.76
5531	O	PHE	B	98	-17.681	-20.276	3.140	1.00	14.57
5532	N	ALA	B	99	-16.804	-19.301	4.957	1.00	14.68
5534	CA	ALA	B	99	-16.424	-18.096	4.217	1.00	14.57
5536	CB	ALA	B	99	-15.730	-17.091	5.134	1.00	14.75
5540	C	ALA	B	99	-15.542	-18.438	3.015	1.00	15.11
5541	O	ALA	B	99	-15.810	-18.017	1.891	1.00	14.86
5542	N	GLU	B	100	-14.505	-19.231	3.255	1.00	15.41
5544	CA	GLU	B	100	-13.580	-19.628	2.203	1.00	16.52
5546	CB	GLU	B	100	-12.418	-20.437	2.793	1.00	17.00
5549	CG	GLU	B	100	-11.436	-20.930	1.735	1.00	20.05
5552	CD	GLU	B	100	-10.193	-21.577	2.315	1.00	23.96
5553	OE1	GLU	B	100	-9.298	-21.933	1.520	1.00	27.94
5554	OE2	GLU	B	100	-10.105	-21.742	3.551	1.00	26.14
5555	C	GLU	B	100	-14.284	-20.439	1.121	1.00	16.30
5556	O	GLU	B	100	-14.115	-20.184	-0.074	1.00	16.61

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
5557	N	GLN	B	101	-15.075	-21.419	1.539	1.00	16.35
5559	CA	GLN	B	101	-15.732	-22.317	0.597	1.00	16.40
5561	CB	GLN	B	101	-16.288	-23.532	1.341	1.00	17.14
5564	CG	GLN	B	101	-15.183	-24.467	1.836	1.00	19.00
5567	CD	GLN	B	101	-15.712	-25.647	2.660	1.00	21.91
5568	OE1	GLN	B	101	-16.894	-25.706	2.993	1.00	25.14
5569	NE2	GLN	B	101	-14.822	-26.583	2.994	1.00	25.16
5572	C	GLN	B	101	-16.829	-21.609	-0.183	1.00	15.19
5573	O	GLN	B	101	-17.079	-21.927	-1.336	1.00	15.71
5574	N	PHE	B	102	-17.461	-20.624	0.444	1.00	14.16
5576	CA	PHE	B	102	-18.476	-19.827	-0.226	1.00	13.43
5578	CB	PHE	B	102	-19.079	-18.788	0.720	1.00	13.06
5581	CG	PHE	B	102	-19.796	-17.694	-0.001	1.00	13.20
5582	CD1	PHE	B	102	-21.010	-17.944	-0.624	1.00	13.03
5584	CE1	PHE	B	102	-21.667	-16.943	-1.322	1.00	14.54
5586	CZ	PHE	B	102	-21.112	-15.673	-1.389	1.00	14.17
5588	CE2	PHE	B	102	-19.913	-15.419	-0.778	1.00	13.73
5590	CD2	PHE	B	102	-19.252	-16.424	-0.084	1.00	12.25
5592	C	PHE	B	102	-17.922	-19.123	-1.457	1.00	13.24
5593	O	PHE	B	102	-18.512	-19.156	-2.524	1.00	13.06
5594	N	VAL	B	103	-16.781	-18.465	-1.299	1.00	13.03
5596	CA	VAL	B	103	-16.202	-17.714	-2.401	1.00	12.67
5598	CB	VAL	B	103	-14.979	-16.901	-1.942	1.00	12.83
5600	CG1	VAL	B	103	-14.271	-16.259	-3.123	1.00	12.54
5604	CG2	VAL	B	103	-15.421	-15.845	-0.960	1.00	12.79
5608	C	VAL	B	103	-15.847	-18.648	-3.547	1.00	12.79
5609	O	VAL	B	103	-16.055	-18.306	-4.708	1.00	12.97
5610	N	ALA	B	104	-15.332	-19.829	-3.216	1.00	12.92
5612	CA	ALA	B	104	-14.948	-20.790	-4.250	1.00	13.56
5614	CB	ALA	B	104	-14.254	-21.970	-3.636	1.00	13.73
5618	C	ALA	B	104	-16.172	-21.241	-5.040	1.00	13.78
5619	O	ALA	B	104	-16.152	-21.272	-6.276	1.00	14.08
5620	N	GLN	B	105	-17.243	-21.560	-4.324	1.00	14.35
5622	CA	GLN	B	105	-18.481	-21.996	-4.964	1.00	15.10
5624	CB	BGLN	B	105	-19.472	-22.606	-3.964	0.35	14.88
5625	CB	AGLN	B	105	-19.439	-22.504	-3.882	0.65	15.24
5630	CG	BGLN	B	105	-20.529	-23.568	-4.585	0.35	15.60
5631	CG	AGLN	B	105	-20.797	-22.994	-4.369	0.65	17.83
5636	CD	BGLN	B	105	-20.104	-24.229	-5.905	0.35	15.35
5637	CD	AGLN	B	105	-21.615	-23.651	-3.256	0.65	20.47
5638	OE1BGLN	B	105		-20.607	-23.872	-6.975	0.35	15.81
5639	OE1AGLN	B	105		-22.763	-24.046	-3.475	0.65	24.49
5640	NE2BGLN	B	105		-19.191	-25.194	-5.828	0.35	15.06
5641	NE2AGLN	B	105		-21.027	-23.761	-2.062	0.65	22.35
5646	C	GLN	B	105	-19.134	-20.873	-5.780	1.00	14.89
5647	O	GLN	B	105	-19.625	-21.113	-6.877	1.00	14.74
5648	N	ALA	B	106	-19.114	-19.644	-5.257	1.00	14.81
5650	CA	ALA	B	106	-19.672	-18.503	-5.972	1.00	14.58
5652	CB	ALA	B	106	-19.631	-17.245	-5.089	1.00	14.32

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
5656	C	ALA	B	106	-18.904	-18.272	-7.277	1.00	15.23
5657	O	ALA	B	106	-19.491	-17.996	-8.320	1.00	15.22
5658	N	GLY	B	107	-17.585	-18.401	-7.204	1.00	15.51
5660	CA	GLY	B	107	-16.720	-18.266	-8.365	1.00	16.19
5663	C	GLY	B	107	-17.008	-19.324	-9.414	1.00	17.13
5664	O	GLY	B	107	-17.044	-19.034	-10.606	1.00	17.74
5665	N	LYS	B	108	-17.248	-20.548	-8.966	1.00	17.91
5667	CA	LYS	B	108	-17.591	-21.645	-9.866	1.00	18.66
5669	CB	LYS	B	108	-17.625	-22.965	-9.093	1.00	19.19
5672	CG	LYS	B	108	-17.783	-24.216	-9.959	1.00	21.83
5675	CD	LYS	B	108	-16.619	-25.192	-9.744	1.00	25.20
5678	CE	LYS	B	108	-16.485	-26.196	-10.884	1.00	26.60
5681	NZ	LYS	B	108	-16.774	-27.581	-10.424	1.00	28.82
5685	C	LYS	B	108	-18.945	-21.412	-10.546	1.00	18.46
5686	O	LYS	B	108	-19.109	-21.708	-11.731	1.00	18.82
5687	N	LEU	B	109	-19.909	-20.885	-9.797	1.00	17.88
5689	CA	LEU	B	109	-21.250	-20.639	-10.329	1.00	18.03
5691	CB	LEU	B	109	-22.219	-20.191	-9.229	1.00	17.95
5694	CG	LEU	B	109	-22.707	-21.232	-8.224	1.00	18.69
5696	CD1	LEU	B	109	-23.375	-20.555	-7.030	1.00	19.02
5700	CD2	LEU	B	109	-23.672	-22.227	-8.883	1.00	20.30
5704	C	LEU	B	109	-21.235	-19.592	-11.435	1.00	17.79
5705	O	LEU	B	109	-21.975	-19.717	-12.404	1.00	18.70
5706	N	MET	B	110	-20.396	-18.568	-11.286	1.00	17.06
5708	CA	MET	B	110	-20.343	-17.454	-12.231	1.00	16.65
5710	CB	MET	B	110	-20.186	-16.135	-11.461	1.00	15.97
5713	CG	MET	B	110	-21.390	-15.788	-10.585	1.00	15.39
5716	SD	MET	B	110	-21.342	-14.125	-9.889	1.00	14.67
5717	CE	MET	B	110	-20.028	-14.328	-8.692	1.00	15.38
5721	C	MET	B	110	-19.230	-17.570	-13.281	1.00	16.48
5722	O	MET	B	110	-19.227	-16.830	-14.263	1.00	17.05
5723	N	GLY	B	111	-18.291	-18.491	-13.090	1.00	16.70
5725	CA	GLY	B	111	-17.129	-18.590	-13.962	1.00	16.57
5728	C	GLY	B	111	-16.127	-17.459	-13.777	1.00	16.53
5729	O	GLY	B	111	-15.483	-17.015	-14.734	1.00	17.27
5730	N	GLY	B	112	-15.993	-17.003	-12.536	1.00	15.78
5732	CA	GLY	B	112	-15.059	-15.950	-12.185	1.00	15.20
5735	C	GLY	B	112	-15.656	-14.946	-11.233	1.00	14.82
5736	O	GLY	B	112	-16.744	-15.146	-10.716	1.00	14.76
5737	N	LEU	B	113	-14.928	-13.860	-11.008	1.00	14.04
5739	CA	LEU	B	113	-15.356	-12.826	-10.070	1.00	13.57
5741	CB	LEU	B	113	-14.963	-13.212	-8.644	1.00	13.54
5744	CG	LEU	B	113	-15.448	-12.269	-7.542	1.00	13.59
5746	CD1	LEU	B	113	-16.952	-12.366	-7.379	1.00	12.89
5750	CD2	LEU	B	113	-14.776	-12.605	-6.233	1.00	13.85
5754	C	LEU	B	113	-14.749	-11.475	-10.431	1.00	13.12
5755	O	LEU	B	113	-13.542	-11.364	-10.600	1.00	13.65
5756	N	ASP	B	114	-15.604	-10.464	-10.553	1.00	12.50
5758	CA	ASP	B	114	-15.203	-9.094	-10.858	1.00	12.77

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
5760	CB	ASP	B	114	-16.082	-8.528	-11.967	1.00	12.87
5763	CG	ASP	B	114	-15.914	-9.263	-13.263	1.00	13.64
5764	OD1	ASP	B	114	-14.780	-9.246	-13.794	1.00	15.61
5765	OD2	ASP	B	114	-16.837	-9.903	-13.817	1.00	15.44
5766	C	ASP	B	114	-15.272	-8.156	-9.659	1.00	12.61
5767	O	ASP	B	114	-14.484	-7.214	-9.562	1.00	12.13
5768	N	MET	B	115	-16.226	-8.388	-8.761	1.00	12.27
5770	CA	MET	B	115	-16.427	-7.512	-7.611	1.00	11.81
5772	CB	MET	B	115	-17.443	-6.413	-7.941	1.00	12.41
5775	CG	MET	B	115	-17.616	-5.388	-6.835	1.00	13.00
5778	SD	MET	B	115	-18.762	-4.058	-7.281	1.00	17.87
5779	CE	MET	B	115	-17.742	-3.072	-8.317	1.00	18.65
5783	C	MET	B	115	-16.884	-8.313	-6.391	1.00	11.51
5784	O	MET	B	115	-17.794	-9.148	-6.484	1.00	11.58
5785	N	LEU	B	116	-16.227	-8.052	-5.267	1.00	11.34
5787	CA	LEU	B	116	-16.539	-8.645	-3.971	1.00	11.05
5789	CB	LEU	B	116	-15.265	-9.238	-3.362	1.00	11.36
5792	CG	LEU	B	116	-15.378	-9.882	-1.980	1.00	11.17
5794	CD1	LEU	B	116	-16.226	-11.139	-2.061	1.00	12.97
5798	CD2	LEU	B	116	-14.015	-10.203	-1.395	1.00	13.15
5802	C	LEU	B	116	-17.082	-7.546	-3.060	1.00	11.06
5803	O	LEU	B	116	-16.335	-6.641	-2.692	1.00	10.73
5804	N	ILE	B	117	-18.373	-7.588	-2.733	1.00	10.99
5806	CA	ILE	B	117	-18.991	-6.577	-1.861	1.00	10.67
5808	CB	ILE	B	117	-20.316	-6.002	-2.456	1.00	10.54
5810	CG1	ILE	B	117	-20.081	-5.440	-3.860	1.00	10.94
5813	CD1	ILE	B	117	-21.333	-4.840	-4.493	1.00	11.34
5817	CG2	ILE	B	117	-20.911	-4.931	-1.532	1.00	11.14
5821	C	ILE	B	117	-19.229	-7.203	-0.485	1.00	10.86
5822	O	ILE	B	117	-20.038	-8.126	-0.331	1.00	10.96
5823	N	LEU	B	118	-18.502	-6.688	0.501	1.00	10.96
5825	CA	LEU	B	118	-18.451	-7.211	1.859	1.00	10.82
5827	CB	LEU	B	118	-17.000	-7.307	2.336	1.00	11.35
5830	CG	LEU	B	118	-16.075	-8.144	1.455	1.00	11.47
5832	CD1	LEU	B	118	-14.612	-8.009	1.873	1.00	13.66
5836	CD2	LEU	B	118	-16.514	-9.611	1.502	1.00	12.89
5840	C	LEU	B	118	-19.273	-6.264	2.724	1.00	10.94
5841	O	LEU	B	118	-18.898	-5.111	2.951	1.00	10.70
5842	N	ASN	B	119	-20.422	-6.758	3.166	1.00	10.94
5844	CA	ASN	B	119	-21.453	-5.914	3.746	1.00	10.66
5846	CB	ASN	B	119	-22.485	-5.681	2.637	1.00	10.88
5849	CG	ASN	B	119	-23.783	-5.129	3.131	1.00	11.09
5850	OD1	ASN	B	119	-24.763	-5.875	3.295	1.00	13.12
5851	ND2	ASN	B	119	-23.839	-3.834	3.327	1.00	8.03
5854	C	ASN	B	119	-22.077	-6.467	5.037	1.00	10.34
5855	O	ASN	B	119	-22.600	-5.695	5.847	1.00	9.93
5856	N	HIS	B	120	-22.024	-7.783	5.245	1.00	9.85
5858	CA	HIS	B	120	-22.611	-8.383	6.448	1.00	10.13
5860	CB	HIS	B	120	-22.518	-9.923	6.396	1.00	10.03

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
5863	CG	HIS	B	120	-21.111	-10.435	6.349	1.00	10.52
5864	ND1	HIS	B	120	-20.355	-10.688	7.469	1.00	13.78
5866	CE1	HIS	B	120	-19.158	-11.108	7.102	1.00	9.73
5868	NE2	HIS	B	120	-19.099	-11.109	5.787	1.00	13.10
5870	CD2	HIS	B	120	-20.301	-10.673	5.295	1.00	9.94
5872	C	HIS	B	120	-22.004	-7.865	7.763	1.00	10.37
5873	O	HIS	B	120	-20.838	-7.495	7.849	1.00	10.29
5874	N	ILE	B	121	-22.820	-7.901	8.807	1.00	10.61
5876	CA	ILE	B	121	-22.386	-7.677	10.183	1.00	11.08
5878	CB	ILE	B	121	-22.633	-6.213	10.652	1.00	11.23
5880	CG1	ILE	B	121	-24.077	-5.787	10.391	1.00	11.88
5883	CD1	ILE	B	121	-24.471	-4.492	11.084	1.00	13.43
5887	CG2	ILE	B	121	-21.647	-5.266	9.988	1.00	12.03
5891	C	ILE	B	121	-23.145	-8.621	11.095	1.00	11.00
5892	O	ILE	B	121	-24.208	-9.112	10.729	1.00	11.76
5893	N	THR	B	122	-22.602	-8.867	12.274	1.00	11.26
5895	CA	THR	B	122	-23.337	-9.597	13.298	1.00	12.09
5897	CB	THR	B	122	-22.363	-10.191	14.358	1.00	12.73
5899	OG1	THR	B	122	-23.048	-11.147	15.179	1.00	13.75
5901	CG2	THR	B	122	-21.834	-9.133	15.314	1.00	12.70
5905	C	THR	B	122	-24.389	-8.670	13.906	1.00	13.10
5906	O	THR	B	122	-24.240	-7.453	13.908	1.00	12.73
5907	N	ASN	B	123	-25.465	-9.248	14.417	1.00	14.53
5909	CA	ASN	B	123	-26.531	-8.439	14.986	1.00	15.80
5911	CB	ASN	B	123	-27.645	-9.315	15.552	1.00	16.12
5914	CG	ASN	B	123	-28.479	-10.012	14.474	1.00	17.74
5915	OD1	ASN	B	123	-28.181	-9.961	13.283	1.00	18.99
5916	ND2	ASN	B	123	-29.537	-10.690	14.913	1.00	22.15
5919	C	ASN	B	123	-25.950	-7.526	16.078	1.00	17.12
5920	O	ASN	B	123	-25.249	-7.988	16.985	1.00	16.93
5921	N	THR	B	124	-26.231	-6.231	15.955	1.00	18.33
5923	CA	THR	B	124	-25.738	-5.203	16.871	1.00	20.06
5925	CB	THR	B	124	-24.552	-4.392	16.242	1.00	20.66
5927	OG1	THR	B	124	-24.357	-3.131	16.908	1.00	23.44
5929	CG2	THR	B	124	-24.799	-3.988	14.807	1.00	20.74
5933	C	THR	B	124	-26.906	-4.293	17.272	1.00	20.70
5934	O	THR	B	124	-27.655	-3.832	16.413	1.00	21.01
5935	N	SER	B	125	-27.066	-4.069	18.572	1.00	20.93
5937	CA	SER	B	125	-27.957	-3.025	19.072	1.00	21.01
5939	CB	SER	B	125	-29.121	-3.649	19.849	1.00	21.06
5942	OG	SER	B	125	-28.691	-4.291	21.018	1.00	22.26
5944	C	SER	B	125	-27.215	-1.997	19.936	1.00	20.65
5945	O	SER	B	125	-26.071	-2.205	20.350	1.00	21.40
5946	N	LEU	B	126	-27.878	-0.879	20.210	1.00	19.36
5948	CA	LEU	B	126	-27.280	0.163	21.025	1.00	18.80
5950	CB	LEU	B	126	-28.030	1.476	20.820	1.00	18.76
5953	CG	LEU	B	126	-28.061	1.969	19.373	1.00	18.94
5955	CD1	LEU	B	126	-28.846	3.267	19.250	1.00	19.67
5959	CD2	LEU	B	126	-26.626	2.148	18.870	1.00	19.43

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
5963	C	LEU	B	126	-27.324	-0.263	22.494	1.00	18.36
5964	O	LEU	B	126	-28.399	-0.481	23.032	1.00	18.29
5965	N	ASN	B	127	-26.161	-0.415	23.125	1.00	17.62
5967	CA	ASN	B	127	-26.077	-0.689	24.572	1.00	17.83
5969	CB	ASN	B	127	-26.203	-2.190	24.894	1.00	18.62
5972	CG	ASN	B	127	-27.400	-2.854	24.245	1.00	21.83
5973	OD1	ASN	B	127	-28.505	-2.846	24.794	1.00	26.41
5974	ND2	ASN	B	127	-27.183	-3.456	23.076	1.00	27.58
5977	C	ASN	B	127	-24.742	-0.228	25.139	1.00	16.87
5978	O	ASN	B	127	-23.733	-0.239	24.425	1.00	15.83
5979	N	LEU	B	128	-24.727	0.132	26.423	1.00	16.44
5981	CA	LEU	B	128	-23.471	0.360	27.144	1.00	17.29
5983	CB	LEU	B	128	-23.728	0.800	28.588	1.00	17.69
5986	CG	LEU	B	128	-24.210	2.227	28.853	1.00	20.16
5988	CD1	LEU	B	128	-24.829	2.299	30.237	1.00	21.49
5992	CD2	LEU	B	128	-23.068	3.208	28.743	1.00	21.98
5996	C	LEU	B	128	-22.673	-0.938	27.174	1.00	17.09
5997	O	LEU	B	128	-23.246	-2.026	27.233	1.00	17.14
5998	N	PHE	B	129	-21.352	-0.820	27.106	1.00	16.64
6000	CA	PHE	B	129	-20.467	-1.969	27.271	1.00	17.36
6002	CB	PHE	B	129	-19.106	-1.722	26.622	1.00	16.86
6005	CG	PHE	B	129	-18.132	-2.850	26.848	1.00	15.42
6006	CD1	PHE	B	129	-18.223	-4.010	26.109	1.00	14.33
6008	CE1	PHE	B	129	-17.337	-5.070	26.341	1.00	13.92
6010	CZ	PHE	B	129	-16.377	-4.960	27.303	1.00	13.02
6012	CE2	PHE	B	129	-16.278	-3.817	28.058	1.00	13.91
6014	CD2	PHE	B	129	-17.164	-2.763	27.840	1.00	14.78
6016	C	PHE	B	129	-20.230	-2.265	28.753	1.00	18.60
6017	O	PHE	B	129	-19.845	-1.380	29.517	1.00	18.70
6018	N	HIS	B	130	-20.415	-3.516	29.147	1.00	20.30
6020	CA	HIS	B	130	-20.118	-3.929	30.517	1.00	21.64
6022	CB	HIS	B	130	-21.410	-4.358	31.221	1.00	22.50
6025	CG	HIS	B	130	-22.346	-3.221	31.483	1.00	24.61
6026	ND1	HIS	B	130	-23.671	-3.238	31.098	1.00	28.31
6028	CE1	HIS	B	130	-24.244	-2.102	31.457	1.00	28.73
6030	NE2	HIS	B	130	-23.337	-1.345	32.048	1.00	28.00
6032	CD2	HIS	B	130	-22.142	-2.022	32.079	1.00	26.84
6034	C	HIS	B	130	-19.044	-5.021	30.564	1.00	22.13
6035	O	HIS	B	130	-17.893	-4.769	30.961	1.00	22.42
6036	N	ASP	B	131	-19.403	-6.226	30.151	1.00	22.71
6038	CA	ASP	B	131	-18.478	-7.345	30.238	1.00	23.07
6040	CB	ASP	B	131	-18.506	-7.939	31.659	1.00	23.40
6043	CG	ASP	B	131	-19.825	-8.628	31.996	1.00	25.28
6044	OD1	ASP	B	131	-20.804	-8.498	31.227	1.00	28.06
6045	OD2	ASP	B	131	-19.978	-9.326	33.030	1.00	28.76
6046	C	ASP	B	131	-18.730	-8.425	29.197	1.00	22.74
6047	O	ASP	B	131	-18.331	-9.568	29.390	1.00	23.32
6048	N	ASP	B	132	-19.354	-8.057	28.080	1.00	22.36
6050	CA	ASP	B	132	-19.740	-9.031	27.070	1.00	21.77



# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
6052	CB	ASP	B	132	-21.028	-8.603	26.346	1.00	22.13
6055	CG	ASP	B	132	-21.705	-9.746	25.621	1.00	23.22
6056	OD1	ASP	B	132	-21.065	-10.797	25.401	1.00	23.84
6057	OD2	ASP	B	132	-22.899	-9.693	25.247	1.00	25.19
6058	C	ASP	B	132	-18.592	-9.175	26.096	1.00	21.19
6059	O	ASP	B	132	-18.657	-8.674	24.971	1.00	19.49
6060	N	ILE	B	133	-17.552	-9.873	26.551	1.00	20.63
6062	CA	ILE	B	133	-16.379	-10.172	25.740	1.00	20.34
6064	CB	ILE	B	133	-15.278	-10.853	26.599	1.00	20.78
6066	CG1	ILE	B	133	-14.840	-9.926	27.745	1.00	22.22
6069	CD1	ILE	B	133	-14.234	-10.631	28.925	1.00	24.20
6073	CG2	ILE	B	133	-14.073	-11.237	25.737	1.00	21.05
6077	C	ILE	B	133	-16.808	-11.089	24.597	1.00	20.10
6078	O	ILE	B	133	-16.230	-11.066	23.518	1.00	18.59
6079	N	HIS	B	134	-17.838	-11.893	24.830	1.00	19.66
6081	CA	HIS	B	134	-18.331	-12.775	23.781	1.00	20.01
6083	CB	BHIS	B	134	-19.438	-13.691	24.321	0.35	20.05
6084	CB	AHIS	B	134	-19.371	-13.733	24.340	0.65	20.50
6089	CG	BHIS	B	134	-20.072	-14.555	23.274	0.35	20.99
6090	CG	AHIS	B	134	-18.820	-14.628	25.405	0.65	22.79
6091	ND1	BHIS	B	134	-21.020	-14.080	22.395	0.35	21.74
6092	ND1	AHIS	B	134	-18.008	-15.705	25.123	0.65	25.14
6095	CE1	BHIS	B	134	-21.392	-15.053	21.584	0.35	21.86
6096	CE1	AHIS	B	134	-17.654	-16.294	26.251	0.65	25.52
6099	NE2	BHIS	B	134	-20.717	-16.142	21.902	0.35	21.70
6100	NE2	AHIS	B	134	-18.190	-15.624	27.256	0.65	26.30
6103	CD2	BHIS	B	134	-19.885	-15.858	22.958	0.35	22.10
6104	CD2	AHIS	B	134	-18.915	-14.571	26.754	0.65	25.17
6107	C	HIS	B	134	-18.844	-11.982	22.581	1.00	18.88
6108	O	HIS	B	134	-18.563	-12.348	21.444	1.00	18.66
6109	N	HIS	B	135	-19.558	-10.889	22.831	1.00	18.30
6111	CA	HIS	B	135	-20.036	-10.022	21.760	1.00	17.67
6113	CB	HIS	B	135	-21.039	-8.997	22.280	1.00	18.39
6116	CG	HIS	B	135	-21.486	-7.998	21.254	1.00	19.37
6117	ND1	HIS	B	135	-22.439	-8.279	20.298	1.00	22.62
6119	CE1	HIS	B	135	-22.639	-7.210	19.552	1.00	22.52
6121	NE2	HIS	B	135	-21.847	-6.246	19.983	1.00	23.50
6123	CD2	HIS	B	135	-21.109	-6.717	21.040	1.00	21.59
6125	C	HIS	B	135	-18.871	-9.307	21.096	1.00	16.64
6126	O	HIS	B	135	-18.876	-9.103	19.889	1.00	16.39
6127	N	VAL	B	136	-17.877	-8.919	21.886	1.00	15.10
6129	CA	VAL	B	136	-16.706	-8.260	21.322	1.00	13.90
6131	CB	VAL	B	136	-15.744	-7.758	22.412	1.00	13.67
6133	CG1	VAL	B	136	-14.516	-7.129	21.776	1.00	13.30
6137	CG2	VAL	B	136	-16.429	-6.746	23.289	1.00	14.14
6141	C	VAL	B	136	-15.984	-9.214	20.366	1.00	13.19
6142	O	VAL	B	136	-15.653	-8.829	19.241	1.00	11.72
6143	N	ARG	B	137	-15.749	-10.449	20.804	1.00	13.24
6145	CA	ARG	B	137	-15.091	-11.436	19.960	1.00	13.70

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
6147	CB	ARG	B	137	-14.782	-12.738	20.703	1.00	14.75
6150	CG	ARG	B	137	-13.868	-13.624	19.877	1.00	16.93
6153	CD	ARG	B	137	-13.649	-15.005	20.405	1.00	21.23
6156	NE	ARG	B	137	-12.360	-15.128	21.070	1.00	25.07
6158	CZ	ARG	B	137	-12.189	-15.046	22.379	1.00	28.33
6159	NH1	ARG	B	137	-13.226	-14.816	23.185	1.00	29.36
6162	NH2	ARG	B	137	-10.973	-15.193	22.893	1.00	28.26
6165	C	ARG	B	137	-15.907	-11.733	18.709	1.00	13.13
6166	O	ARG	B	137	-15.362	-11.777	17.611	1.00	12.08
6167	N	LYS	B	138	-17.212	-11.920	18.872	1.00	13.25
6169	CA	LYS	B	138	-18.061	-12.268	17.740	1.00	13.63
6171	CB	LYS	B	138	-19.475	-12.622	18.202	1.00	14.03
6174	CG	LYS	B	138	-20.354	-13.165	17.079	1.00	16.95
6177	CD	LYS	B	138	-21.750	-13.472	17.571	1.00	19.47
6180	CE	LYS	B	138	-21.821	-14.813	18.233	1.00	22.59
6183	NZ	LYS	B	138	-23.212	-15.073	18.710	1.00	25.93
6187	C	LYS	B	138	-18.109	-11.131	16.733	1.00	13.03
6188	O	LYS	B	138	-18.111	-11.366	15.524	1.00	13.21
6189	N	SER	B	139	-18.118	-9.902	17.228	1.00	12.83
6191	CA	SER	B	139	-18.080	-8.741	16.349	1.00	12.66
6193	CB	SER	B	139	-18.203	-7.447	17.154	1.00	13.29
6196	OG	SER	B	139	-19.492	-7.350	17.746	1.00	14.95
6198	C	SER	B	139	-16.792	-8.734	15.552	1.00	12.54
6199	O	SER	B	139	-16.803	-8.484	14.338	1.00	12.28
6200	N	MET	B	140	-15.680	-9.005	16.225	1.00	12.60
6202	CA	MET	B	140	-14.395	-8.978	15.556	1.00	12.80
6204	CB	MET	B	140	-13.235	-9.057	16.554	1.00	13.25
6207	CG	MET	B	140	-13.012	-7.828	17.434	1.00	16.23
6210	SD	MET	B	140	-12.919	-6.194	16.580	1.00	21.70
6211	CE	MET	B	140	-12.095	-6.717	15.058	1.00	14.36
6215	C	MET	B	140	-14.325	-10.107	14.526	1.00	12.58
6216	O	MET	B	140	-13.812	-9.919	13.424	1.00	12.83
6217	N	GLU	B	141	-14.903	-11.267	14.844	1.00	12.10
6219	CA	GLU	B	141	-14.819	-12.415	13.940	1.00	12.43
6221	CB	GLU	B	141	-15.151	-13.719	14.675	1.00	12.80
6224	CG	GLU	B	141	-14.069	-14.185	15.646	1.00	15.61
6227	CD	GLU	B	141	-12.943	-14.945	14.970	1.00	21.48
6228	OE1	GLU	B	141	-11.782	-14.827	15.422	1.00	25.76
6229	OE2	GLU	B	141	-13.209	-15.684	13.997	1.00	26.71
6230	C	GLU	B	141	-15.724	-12.234	12.719	1.00	11.67
6231	O	GLU	B	141	-15.301	-12.417	11.583	1.00	12.21
6232	N	VAL	B	142	-16.974	-11.836	12.947	1.00	11.25
6234	CA	VAL	B	142	-17.927	-11.713	11.855	1.00	11.22
6236	CB	VAL	B	142	-19.370	-11.773	12.364	1.00	10.62
6238	CG1	VAL	B	142	-20.358	-11.520	11.249	1.00	11.29
6242	CG2	VAL	B	142	-19.635	-13.128	13.015	1.00	11.47
6246	C	VAL	B	142	-17.720	-10.436	11.048	1.00	10.72
6247	O	VAL	B	142	-17.721	-10.472	9.816	1.00	11.69
6248	N	ASN	B	143	-17.534	-9.313	11.723	1.00	10.27

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
6250	CA	ASN	B	143	-17.486	-8.021	11.036	1.00	9.98
6252	CB	ASN	B	143	-17.788	-6.873	11.986	1.00	9.71
6255	CG	ASN	B	143	-19.150	-6.948	12.603	1.00	10.65
6256	OD1	ASN	B	143	-19.964	-7.839	12.300	1.00	9.89
6257	ND2	ASN	B	143	-19.407	-6.012	13.522	1.00	11.96
6260	C	ASN	B	143	-16.134	-7.709	10.401	1.00	9.99
6261	O	ASN	B	143	-16.068	-6.870	9.497	1.00	11.03
6262	N	PHE	B	144	-15.068	-8.350	10.903	1.00	10.09
6264	CA	PHE	B	144	-13.698	-8.033	10.484	1.00	10.06
6266	CB	PHE	B	144	-12.880	-7.377	11.606	1.00	9.97
6269	CG	PHE	B	144	-11.420	-7.287	11.283	1.00	10.21
6270	CD1	PHE	B	144	-11.003	-6.484	10.249	1.00	11.64
6272	CE1	PHE	B	144	-9.673	-6.420	9.899	1.00	12.65
6274	CZ	PHE	B	144	-8.749	-7.186	10.559	1.00	11.94
6276	CE2	PHE	B	144	-9.135	-8.002	11.584	1.00	11.08
6278	CD2	PHE	B	144	-10.490	-8.069	11.941	1.00	10.76
6280	C	PHE	B	144	-12.966	-9.265	9.946	1.00	10.00
6281	O	PHE	B	144	-12.627	-9.299	8.773	1.00	10.10
6282	N	LEU	B	145	-12.744	-10.285	10.767	1.00	10.14
6284	CA	LEU	B	145	-11.915	-11.411	10.309	1.00	10.57
6286	CB	BLEU	B	145	-11.636	-12.402	11.446	0.35	10.78
6287	CB	ALEU	B	145	-11.663	-12.396	11.456	0.65	10.84
6292	CG	BLEU	B	145	-10.504	-11.991	12.390	0.35	11.79
6293	CG	ALEU	B	145	-10.559	-13.423	11.214	0.65	12.14
6296	CD1BLEU	B	145		-10.429	-12.962	13.541	0.35	13.06
6297	CD1ALEU	B	145		-9.201	-12.766	11.048	0.65	12.48
6304	CD2BLEU	B	145		-9.168	-11.911	11.672	0.35	12.39
6305	CD2ALEU	B	145		-10.553	-14.386	12.373	0.65	12.74
6312	C	LEU	B	145	-12.518	-12.132	9.102	1.00	10.24
6313	O	LEU	B	145	-11.792	-12.502	8.173	1.00	10.28
6314	N	SER	B	146	-13.842	-12.300	9.064	1.00	9.84
6316	CA	SER	B	146	-14.450	-12.956	7.915	1.00	9.89
6318	CB	SER	B	146	-15.934	-13.267	8.129	1.00	9.62
6321	OG	SER	B	146	-16.725	-12.091	8.059	1.00	10.58
6323	C	SER	B	146	-14.231	-12.157	6.638	1.00	9.60
6324	O	SER	B	146	-14.111	-12.743	5.568	1.00	10.67
6325	N	TYR	B	147	-14.175	-10.825	6.728	1.00	9.77
6327	CA	TYR	B	147	-13.891	-10.018	5.543	1.00	10.01
6329	CB	TYR	B	147	-13.990	-8.512	5.818	1.00	10.11
6332	CG	TYR	B	147	-15.404	-7.920	5.917	1.00	9.31
6333	CD1	TYR	B	147	-16.484	-8.637	6.450	1.00	10.54
6335	CE1	TYR	B	147	-17.755	-8.058	6.544	1.00	10.91
6337	CZ	TYR	B	147	-17.958	-6.771	6.091	1.00	10.19
6338	OH	TYR	B	147	-19.214	-6.196	6.192	1.00	11.05
6340	CE2	TYR	B	147	-16.899	-6.047	5.553	1.00	9.46
6342	CD2	TYR	B	147	-15.646	-6.622	5.474	1.00	9.21
6344	C	TYR	B	147	-12.500	-10.332	5.009	1.00	10.15
6345	O	TYR	B	147	-12.297	-10.370	3.810	1.00	10.88
6346	N	VAL	B	148	-11.546	-10.541	5.912	1.00	10.24

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
6348	CA	VAL	B	148	-10.179	-10.882	5.512	1.00	10.73
6350	CB	VAL	B	148	-9.204	-10.789	6.705	1.00	10.37
6352	CG1	VAL	B	148	-9.247	-9.396	7.318	1.00	11.74
6356	CG2	VAL	B	148	-7.782	-11.137	6.260	1.00	11.68
6360	C	VAL	B	148	-10.150	-12.260	4.843	1.00	10.43
6361	O	VAL	B	148	-9.545	-12.437	3.782	1.00	10.90
6362	N	VAL	B	149	-10.839	-13.226	5.441	1.00	10.89
6364	CA	VAL	B	149	-10.904	-14.567	4.882	1.00	11.04
6366	CB	VAL	B	149	-11.670	-15.522	5.808	1.00	11.48
6368	CG1	VAL	B	149	-11.877	-16.876	5.131	1.00	11.08
6372	CG2	VAL	B	149	-10.946	-15.687	7.131	1.00	12.02
6376	C	VAL	B	149	-11.531	-14.541	3.487	1.00	11.11
6377	O	VAL	B	149	-11.040	-15.203	2.566	1.00	11.58
6378	N	LEU	B	150	-12.625	-13.794	3.332	1.00	10.60
6380	CA	LEU	B	150	-13.305	-13.692	2.052	1.00	10.56
6382	CB	LEU	B	150	-14.597	-12.880	2.215	1.00	10.24
6385	CG	LEU	B	150	-15.686	-13.601	2.996	1.00	11.43
6387	CD1	LEU	B	150	-16.712	-12.580	3.499	1.00	10.46
6391	CD2	LEU	B	150	-16.367	-14.699	2.188	1.00	12.15
6395	C	LEU	B	150	-12.403	-13.070	0.998	1.00	10.64
6396	O	LEU	B	150	-12.373	-13.501	-0.153	1.00	10.72
6397	N	THR	B	151	-11.671	-12.042	1.402	1.00	11.03
6399	CA	THR	B	151	-10.739	-11.368	0.517	1.00	11.66
6401	CB	THR	B	151	-10.164	-10.133	1.222	1.00	11.70
6403	OG1	THR	B	151	-11.212	-9.169	1.415	1.00	12.53
6405	CG2	THR	B	151	-9.128	-9.416	0.347	1.00	13.92
6409	C	THR	B	151	-9.637	-12.308	0.052	1.00	11.60
6410	O	THR	B	151	-9.321	-12.349	-1.133	1.00	12.25
6411	N	VAL	B	152	-9.063	-13.072	0.967	1.00	10.91
6413	CA	VAL	B	152	-8.004	-14.014	0.607	1.00	11.09
6415	CB	VAL	B	152	-7.458	-14.710	1.874	1.00	11.31
6417	CG1	VAL	B	152	-6.630	-15.919	1.514	1.00	12.41
6421	CG2	VAL	B	152	-6.639	-13.724	2.702	1.00	11.67
6425	C	VAL	B	152	-8.512	-15.037	-0.413	1.00	11.04
6426	O	VAL	B	152	-7.826	-15.349	-1.402	1.00	12.04
6427	N	ALA	B	153	-9.716	-15.537	-0.179	1.00	11.23
6429	CA	ALA	B	153	-10.354	-16.507	-1.070	1.00	11.42
6431	CB	ALA	B	153	-11.635	-17.013	-0.444	1.00	11.88
6435	C	ALA	B	153	-10.633	-15.917	-2.449	1.00	11.72
6436	O	ALA	B	153	-10.584	-16.626	-3.448	1.00	12.33
6437	N	ALA	B	154	-10.974	-14.637	-2.500	1.00	11.17
6439	CA	ALA	B	154	-11.416	-13.997	-3.738	1.00	11.57
6441	CB	ALA	B	154	-12.382	-12.869	-3.422	1.00	12.27
6445	C	ALA	B	154	-10.265	-13.447	-4.565	1.00	11.52
6446	O	ALA	B	154	-10.415	-13.209	-5.766	1.00	11.61
6447	N	LEU	B	155	-9.133	-13.189	-3.928	1.00	12.01
6449	CA	LEU	B	155	-8.102	-12.383	-4.579	1.00	12.40
6451	CB	LEU	B	155	-6.957	-12.017	-3.623	1.00	12.53
6454	CG	LEU	B	155	-6.019	-10.910	-4.122	1.00	15.17

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
6456	CD1	LEU	B	155	-4.872	-10.735	-3.139	1.00	17.34
6460	CD2	LEU	B	155	-6.727	-9.588	-4.376	1.00	16.49
6464	C	LEU	B	155	-7.575	-12.982	-5.891	1.00	12.20
6465	O	LEU	B	155	-7.423	-12.236	-6.856	1.00	11.65
6466	N	PRO	B	156	-7.287	-14.283	-5.971	1.00	12.56
6467	CA	PRO	B	156	-6.824	-14.838	-7.250	1.00	12.74
6469	CB	PRO	B	156	-6.681	-16.331	-6.956	1.00	12.66
6472	CG	PRO	B	156	-6.418	-16.378	-5.513	1.00	12.78
6475	CD	PRO	B	156	-7.302	-15.312	-4.917	1.00	13.15
6478	C	PRO	B	156	-7.780	-14.555	-8.416	1.00	12.90
6479	O	PRO	B	156	-7.310	-14.172	-9.491	1.00	13.46
6480	N	MET	B	157	-9.085	-14.698	-8.195	1.00	12.50
6482	CA	MET	B	157	-10.079	-14.383	-9.215	1.00	12.50
6484	CB	MET	B	157	-11.473	-14.878	-8.799	1.00	12.82
6487	CG	MET	B	157	-11.661	-16.369	-8.979	1.00	13.70
6490	SD	MET	B	157	-13.345	-16.928	-8.707	1.00	16.97
6491	CE	MET	B	157	-13.494	-16.728	-6.948	1.00	15.98
6495	C	MET	B	157	-10.126	-12.892	-9.538	1.00	12.28
6496	O	MET	B	157	-10.277	-12.513	-10.699	1.00	12.48
6497	N	LEU	B	158	-10.012	-12.046	-8.516	1.00	12.06
6499	CA	LEU	B	158	-9.988	-10.600	-8.723	1.00	11.94
6501	CB	LEU	B	158	-10.151	-9.856	-7.402	1.00	11.86
6504	CG	LEU	B	158	-11.477	-10.107	-6.670	1.00	11.77
6506	CD1	LEU	B	158	-11.428	-9.484	-5.268	1.00	13.32
6510	CD2	LEU	B	158	-12.655	-9.578	-7.466	1.00	12.74
6514	C	LEU	B	158	-8.719	-10.139	-9.450	1.00	12.20
6515	O	LEU	B	158	-8.781	-9.212	-10.230	1.00	12.72
6516	N	LYS	B	159	-7.592	-10.801	-9.224	1.00	12.72
6518	CA	LYS	B	159	-6.366	-10.459	-9.949	1.00	13.55
6520	CB	LYS	B	159	-5.150	-11.160	-9.338	1.00	13.65
6523	CG	LYS	B	159	-4.675	-10.532	-8.046	1.00	14.07
6526	CD	LYS	B	159	-3.698	-11.422	-7.300	1.00	15.40
6529	CE	LYS	B	159	-2.983	-10.659	-6.207	1.00	16.67
6532	NZ	LYS	B	159	-2.057	-11.539	-5.405	1.00	19.28
6536	C	LYS	B	159	-6.537	-10.814	-11.423	1.00	14.46
6537	O	LYS	B	159	-6.063	-10.092	-12.310	1.00	15.16
6538	N	Gln	B	160	-7.236	-11.912	-11.696	1.00	15.28
6540	CA	Gln	B	160	-7.489	-12.331	-13.072	1.00	16.39
6542	CB	Gln	B	160	-8.185	-13.695	-13.098	1.00	16.89
6545	CG	Gln	B	160	-7.328	-14.858	-12.668	1.00	20.04
6548	CD	Gln	B	160	-8.105	-16.166	-12.691	1.00	23.99
6549	OE1	Gln	B	160	-8.376	-16.708	-13.765	1.00	29.36
6550	NE2	Gln	B	160	-8.491	-16.662	-11.515	1.00	25.62
6553	C	Gln	B	160	-8.331	-11.316	-13.834	1.00	16.16
6554	O	Gln	B	160	-8.092	-11.066	-15.016	1.00	17.01
6555	N	SER	B	161	-9.291	-10.703	-13.143	1.00	15.38
6557	CA	SER	B	161	-10.235	-9.781	-13.769	1.00	14.97
6559	CB	SER	B	161	-11.631	-10.046	-13.221	1.00	15.47
6562	OG	SER	B	161	-11.666	-9.816	-11.826	1.00	14.66

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
6564	C	SER	B	161	-9.907	-8.301	-13.563	1.00	14.44
6565	O	SER	B	161	-10.672	-7.436	-14.011	1.00	14.01
6566	N	ASN	B	162	-8.787	-8.005	-12.899	1.00	14.05
6568	CA	ASN	B	162	-8.493	-6.629	-12.458	1.00	14.12
6570	CB	ASN	B	162	-8.111	-5.731	-13.631	1.00	14.73
6573	CG	ASN	B	162	-6.944	-6.280	-14.425	1.00	17.47
6574	OD1	ASN	B	162	-5.858	-6.471	-13.889	1.00	20.39
6575	ND2	ASN	B	162	-7.166	-6.533	-15.713	1.00	22.34
6578	C	ASN	B	162	-9.700	-6.040	-11.744	1.00	13.54
6579	O	ASN	B	162	-10.167	-4.941	-12.066	1.00	13.29
6580	N	GLY	B	163	-10.200	-6.800	-10.776	1.00	12.77
6582	CA	GLY	B	163	-11.468	-6.533	-10.140	1.00	12.40
6585	C	GLY	B	163	-11.394	-5.588	-8.962	1.00	12.14
6586	O	GLY	B	163	-10.469	-4.799	-8.833	1.00	10.92
6587	N	SER	B	164	-12.386	-5.709	-8.088	1.00	12.40
6589	CA	SER	B	164	-12.657	-4.716	-7.063	1.00	12.29
6591	CB	SER	B	164	-13.675	-3.711	-7.604	1.00	12.63
6594	OG	SER	B	164	-13.190	-3.090	-8.783	1.00	15.53
6596	C	SER	B	164	-13.209	-5.337	-5.795	1.00	11.77
6597	O	SER	B	164	-14.020	-6.263	-5.845	1.00	12.29
6598	N	ILE	B	165	-12.760	-4.804	-4.669	1.00	10.79
6600	CA	ILE	B	165	-13.257	-5.136	-3.348	1.00	10.81
6602	CB	ILE	B	165	-12.103	-5.536	-2.422	1.00	11.35
6604	CG1	ILE	B	165	-11.351	-6.735	-2.983	1.00	12.49
6607	CD1	ILE	B	165	-9.968	-6.920	-2.362	1.00	15.04
6611	CG2	ILE	B	165	-12.641	-5.827	-1.025	1.00	12.62
6615	C	ILE	B	165	-13.950	-3.907	-2.788	1.00	10.55
6616	O	ILE	B	165	-13.384	-2.818	-2.788	1.00	10.14
6617	N	VAL	B	166	-15.170	-4.088	-2.298	1.00	10.31
6619	CA	VAL	B	166	-15.942	-3.021	-1.693	1.00	10.44
6621	CB	VAL	B	166	-17.271	-2.772	-2.437	1.00	10.79
6623	CG1	VAL	B	166	-18.079	-1.672	-1.749	1.00	12.71
6627	CG2	VAL	B	166	-16.992	-2.419	-3.881	1.00	11.11
6631	C	VAL	B	166	-16.214	-3.433	-0.263	1.00	10.36
6632	O	VAL	B	166	-16.777	-4.509	-0.012	1.00	10.73
6633	N	VAL	B	167	-15.770	-2.606	0.670	1.00	10.27
6635	CA	VAL	B	167	-15.926	-2.849	2.104	1.00	10.60
6637	CB	VAL	B	167	-14.555	-2.767	2.832	1.00	10.54
6639	CG1	VAL	B	167	-14.724	-2.936	4.339	1.00	11.91
6643	CG2	VAL	B	167	-13.599	-3.811	2.281	1.00	13.18
6647	C	VAL	B	167	-16.885	-1.813	2.690	1.00	10.88
6648	O	VAL	B	167	-16.612	-0.621	2.651	1.00	10.80
6649	N	VAL	B	168	-18.010	-2.284	3.230	1.00	10.31
6651	CA	VAL	B	168	-19.035	-1.400	3.781	1.00	10.54
6653	CB	VAL	B	168	-20.475	-1.944	3.575	1.00	10.54
6655	CG1	VAL	B	168	-21.500	-0.928	4.056	1.00	10.55
6659	CG2	VAL	B	168	-20.715	-2.249	2.108	1.00	10.42
6663	C	VAL	B	168	-18.738	-1.129	5.257	1.00	10.84
6664	O	VAL	B	168	-18.599	-2.046	6.066	1.00	11.28

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
6665	N	SER	B	169	-18.620	0.154	5.567	1.00	10.80
6667	CA	SER	B	169	-18.340	0.634	6.912	1.00	10.94
6669	CB	SER	B	169	-16.866	1.013	7.062	1.00	10.92
6672	OG	SER	B	169	-16.539	1.221	8.434	1.00	12.02
6674	C	SER	B	169	-19.276	1.802	7.242	1.00	11.06
6675	O	SER	B	169	-20.375	1.906	6.695	1.00	11.35
6676	N	SER	B	170	-18.841	2.680	8.133	1.00	10.47
6678	CA	SER	B	170	-19.768	3.360	9.033	1.00	10.20
6680	CB	SER	B	170	-20.057	2.457	10.245	1.00	10.68
6683	OG	SER	B	170	-20.316	1.135	9.837	1.00	11.35
6685	C	SER	B	170	-19.177	4.643	9.554	1.00	9.92
6686	O	SER	B	170	-17.965	4.741	9.722	1.00	10.64
6687	N	LEU	B	171	-20.024	5.613	9.880	1.00	9.43
6689	CA	LEU	B	171	-19.539	6.765	10.646	1.00	9.32
6691	CB	LEU	B	171	-20.683	7.709	11.036	1.00	9.63
6694	CG	LEU	B	171	-21.317	8.485	9.875	1.00	10.60
6696	CD1	LEU	B	171	-20.317	9.408	9.182	1.00	13.36
6700	CD2	LEU	B	171	-22.482	9.277	10.404	1.00	10.91
6704	C	LEU	B	171	-18.800	6.307	11.904	1.00	9.27
6705	O	LEU	B	171	-17.779	6.886	12.258	1.00	9.16
6706	N	ALA	B	172	-19.305	5.269	12.573	1.00	9.43
6708	CA	ALA	B	172	-18.681	4.742	13.792	1.00	9.90
6710	CB	ALA	B	172	-19.697	3.930	14.604	1.00	10.25
6714	C	ALA	B	172	-17.427	3.904	13.489	1.00	10.34
6715	O	ALA	B	172	-16.815	3.345	14.401	1.00	10.61
6716	N	GLY	B	173	-17.054	3.841	12.208	1.00	9.97
6718	CA	GLY	B	173	-15.771	3.333	11.764	1.00	10.16
6721	C	GLY	B	173	-14.752	4.415	11.424	1.00	10.15
6722	O	GLY	B	173	-13.647	4.095	10.973	1.00	9.80
6723	N	LYS	B	174	-15.117	5.679	11.655	1.00	9.63
6725	CA	LYS	B	174	-14.239	6.838	11.411	1.00	10.00
6727	CB	LYS	B	174	-14.716	7.637	10.180	1.00	9.93
6730	CG	LYS	B	174	-14.516	6.920	8.855	1.00	10.50
6733	CD	LYS	B	174	-13.044	6.724	8.522	1.00	10.16
6736	CE	LYS	B	174	-12.829	6.393	7.066	1.00	10.53
6739	NZ	LYS	B	174	-11.360	6.286	6.773	1.00	10.87
6743	C	LYS	B	174	-14.143	7.768	12.619	1.00	10.23
6744	O	LYS	B	174	-13.119	8.440	12.811	1.00	10.55
6745	N	VAL	B	175	-15.214	7.862	13.392	1.00	10.53
6747	CA	VAL	B	175	-15.215	8.602	14.651	1.00	10.47
6749	CB	VAL	B	175	-15.903	9.971	14.523	1.00	10.86
6751	CG1	VAL	B	175	-17.403	9.829	14.318	1.00	12.39
6755	CG2	VAL	B	175	-15.250	10.768	13.384	1.00	10.43
6759	C	VAL	B	175	-15.868	7.752	15.734	1.00	10.34
6760	O	VAL	B	175	-16.515	6.728	15.444	1.00	10.95
6761	N	ALA	B	176	-15.690	8.169	16.975	1.00	11.24
6763	CA	ALA	B	176	-16.190	7.405	18.118	1.00	11.39
6765	CB	ALA	B	176	-15.226	7.500	19.273	1.00	11.50
6769	C	ALA	B	176	-17.588	7.806	18.577	1.00	11.40

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
6770	O	ALA	B	176	-17.942	8.986	18.620	1.00	12.07
6771	N	TYR	B	177	-18.374	6.794	18.944	1.00	10.95
6773	CA	TYR	B	177	-19.714	6.977	19.490	1.00	11.62
6775	CB	TYR	B	177	-20.766	6.506	18.487	1.00	11.73
6778	CG	TYR	B	177	-20.956	7.363	17.270	1.00	10.76
6779	CD1	TYR	B	177	-20.118	7.228	16.175	1.00	11.13
6781	CE1	TYR	B	177	-20.288	7.991	15.042	1.00	11.25
6783	CZ	TYR	B	177	-21.311	8.916	14.991	1.00	10.66
6784	OH	TYR	B	177	-21.472	9.665	13.852	1.00	11.56
6786	CE2	TYR	B	177	-22.158	9.074	16.056	1.00	11.13
6788	CD2	TYR	B	177	-21.986	8.289	17.194	1.00	11.28
6790	C	TYR	B	177	-19.876	6.077	20.702	1.00	11.37
6791	O	TYR	B	177	-19.401	4.944	20.684	1.00	11.93
6792	N	PRO	B	178	-20.626	6.507	21.704	1.00	11.55
6793	CA	PRO	B	178	-21.017	5.587	22.772	1.00	11.93
6795	CB	PRO	B	178	-21.627	6.504	23.825	1.00	11.95
6798	CG	PRO	B	178	-22.167	7.653	23.042	1.00	11.98
6801	CD	PRO	B	178	-21.254	7.831	21.861	1.00	11.86
6804	C	PRO	B	178	-22.062	4.594	22.248	1.00	11.98
6805	O	PRO	B	178	-22.723	4.847	21.248	1.00	12.48
6806	N	MET	B	179	-22.188	3.473	22.947	1.00	12.17
6808	CA	MET	B	179	-23.224	2.444	22.757	1.00	12.36
6810	CB	BMET	B	179	-24.633	3.029	22.495	0.35	12.42
6811	CG	AMET	B	179	-24.630	3.067	22.664	0.65	13.16
6816	CB	BMET	B	179	-25.055	4.271	23.253	0.35	12.59
6817	CG	AMET	B	179	-24.956	4.066	23.789	0.65	15.42
6822	SD	BMET	B	179	-26.674	4.858	22.660	0.35	12.77
6823	SD	AMET	B	179	-24.457	3.555	25.461	0.65	20.19
6824	CE	BMET	B	179	-27.213	5.684	24.020	0.35	14.60
6825	CE	AMET	B	179	-24.896	4.938	26.456	0.65	21.28
6832	C	MET	B	179	-22.944	1.461	21.613	1.00	11.78
6833	O	MET	B	179	-23.747	0.559	21.368	1.00	12.41
6834	N	VAL	B	180	-21.817	1.636	20.917	1.00	10.61
6836	CA	VAL	B	180	-21.448	0.772	19.800	1.00	10.87
6838	CB	VAL	B	180	-21.767	1.429	18.426	1.00	11.08
6840	CG1	VAL	B	180	-23.269	1.474	18.191	1.00	12.20
6844	CG2	VAL	B	180	-21.140	2.809	18.315	1.00	12.39
6848	C	VAL	B	180	-19.959	0.382	19.869	1.00	10.10
6849	O	VAL	B	180	-19.294	0.270	18.844	1.00	11.08
6850	N	ALA	B	181	-19.436	0.158	21.067	1.00	10.18
6852	CA	ALA	B	181	-17.978	-0.030	21.247	1.00	10.20
6854	CB	ALA	B	181	-17.621	-0.135	22.729	1.00	10.67
6858	C	ALA	B	181	-17.418	-1.225	20.471	1.00	9.89
6859	O	ALA	B	181	-16.440	-1.077	19.740	1.00	9.82
6860	N	ALA	B	182	-18.022	-2.404	20.633	1.00	9.30
6862	CA	ALA	B	182	-17.560	-3.607	19.925	1.00	9.47
6864	CB	ALA	B	182	-18.362	-4.798	20.362	1.00	9.82
6868	C	ALA	B	182	-17.661	-3.449	18.413	1.00	9.76
6869	O	ALA	B	182	-16.763	-3.840	17.667	1.00	10.64



# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
6870	N	TYR	B	183	-18.766	-2.875	17.946	1.00	9.09
6872	CA	TYR	B	183	-18.970	-2.653	16.521	1.00	9.39
6874	CB	TYR	B	183	-20.362	-2.091	16.307	1.00	9.89
6877	CG	TYR	B	183	-20.697	-1.582	14.930	1.00	9.36
6878	CD1	TYR	B	183	-21.250	-2.421	13.973	1.00	8.46
6880	CE1	TYR	B	183	-21.595	-1.955	12.721	1.00	8.81
6882	CZ	TYR	B	183	-21.437	-0.621	12.415	1.00	9.45
6883	OH	TYR	B	183	-21.833	-0.136	11.192	1.00	11.31
6885	CE2	TYR	B	183	-20.872	0.237	13.346	1.00	10.50
6887	CD2	TYR	B	183	-20.515	-0.240	14.595	1.00	8.78
6889	C	TYR	B	183	-17.949	-1.678	15.977	1.00	9.38
6890	O	TYR	B	183	-17.369	-1.905	14.919	1.00	9.47
6891	N	SER	B	184	-17.754	-0.580	16.689	1.00	9.95
6893	CA	SER	B	184	-16.801	0.435	16.267	1.00	10.14
6895	CB	SER	B	184	-16.824	1.622	17.220	1.00	11.38
6898	OG	SER	B	184	-15.894	2.602	16.828	1.00	16.20
6900	C	SER	B	184	-15.394	-0.148	16.170	1.00	9.89
6901	O	SER	B	184	-14.698	0.133	15.217	1.00	9.45
6902	N	ALA	B	185	-15.006	-0.978	17.132	1.00	9.56
6904	CA	ALA	B	185	-13.696	-1.643	17.060	1.00	9.45
6906	CB	ALA	B	185	-13.475	-2.551	18.215	1.00	9.09
6910	C	ALA	B	185	-13.567	-2.403	15.761	1.00	9.17
6911	O	ALA	B	185	-12.531	-2.304	15.090	1.00	8.89
6912	N	SER	B	186	-14.605	-3.149	15.383	1.00	8.39
6914	CA	SER	B	186	-14.534	-3.955	14.168	1.00	8.65
6916	CB	SER	B	186	-15.677	-4.965	14.094	1.00	8.65
6919	OG	SER	B	186	-16.932	-4.356	13.840	1.00	9.10
6921	C	SER	B	186	-14.454	-3.115	12.904	1.00	8.69
6922	O	SER	B	186	-13.738	-3.474	11.969	1.00	9.00
6923	N	LYS	B	187	-15.171	-1.995	12.860	1.00	8.31
6925	CA	LYS	B	187	-15.178	-1.150	11.665	1.00	8.18
6927	CB	LYS	B	187	-16.413	-0.241	11.645	1.00	8.67
6930	CG	LYS	B	187	-17.749	-0.998	11.530	1.00	8.98
6933	CD	LYS	B	187	-17.837	-1.815	10.238	1.00	8.83
6936	CE	LYS	B	187	-19.274	-2.175	9.865	1.00	10.34
6939	NZ	LYS	B	187	-19.399	-2.928	8.581	1.00	8.88
6943	C	LYS	B	187	-13.881	-0.330	11.552	1.00	7.85
6944	O	LYS	B	187	-13.358	-0.128	10.460	1.00	8.40
6945	N	PHE	B	188	-13.382	0.161	12.672	1.00	8.19
6947	CA	PHE	B	188	-12.053	0.764	12.709	1.00	7.78
6949	CB	PHE	B	188	-11.692	1.235	14.122	1.00	7.54
6952	CG	PHE	B	188	-12.081	2.669	14.429	1.00	7.84
6953	CD1	PHE	B	188	-11.101	3.626	14.630	1.00	8.16
6955	CE1	PHE	B	188	-11.433	4.943	14.941	1.00	8.44
6957	CZ	PHE	B	188	-12.742	5.322	15.056	1.00	8.30
6959	CE2	PHE	B	188	-13.752	4.352	14.876	1.00	7.99
6961	CD2	PHE	B	188	-13.408	3.044	14.560	1.00	8.33
6963	C	PHE	B	188	-11.011	-0.247	12.195	1.00	7.71
6964	O	PHE	B	188	-10.138	0.120	11.394	1.00	8.02

## FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
6965	N	ALA	B	189	-11.112	-1.509	12.617	1.00	7.76
6967	CA	ALA	B	189	-10.165	-2.544	12.178	1.00	8.36
6969	CB	ALA	B	189	-10.462	-3.851	12.849	1.00	8.12
6973	C	ALA	B	189	-10.187	-2.710	10.659	1.00	8.84
6974	O	ALA	B	189	-9.140	-2.831	10.044	1.00	8.96
6975	N	LEU	B	190	-11.377	-2.691	10.058	1.00	8.73
6977	CA	LEU	B	190	-11.505	-2.771	8.607	1.00	9.25
6979	CB	LEU	B	190	-12.982	-2.718	8.193	1.00	9.20
6982	CG	LEU	B	190	-13.817	-3.958	8.470	1.00	10.50
6984	CD1	LEU	B	190	-15.268	-3.629	8.170	1.00	11.23
6988	CD2	LEU	B	190	-13.330	-5.138	7.637	1.00	10.76
6992	C	LEU	B	190	-10.750	-1.642	7.907	1.00	9.46
6993	O	LEU	B	190	-10.103	-1.864	6.891	1.00	9.36
6994	N	ASP	B	191	-10.834	-0.433	8.440	1.00	9.39
6996	CA	ASP	B	191	-10.131	0.706	7.852	1.00	9.69
6998	CB	ASP	B	191	-10.544	1.972	8.583	1.00	9.68
7001	CG	ASP	B	191	-10.029	3.233	7.948	1.00	10.57
7002	OD1	ASP	B	191	-9.398	3.195	6.869	1.00	11.55
7003	OD2	ASP	B	191	-10.235	4.331	8.493	1.00	11.12
7004	C	ASP	B	191	-8.618	0.467	7.920	1.00	9.64
7005	O	ASP	B	191	-7.911	0.572	6.921	1.00	10.14
7006	N	GLY	B	192	-8.121	0.129	9.104	1.00	10.15
7008	CA	GLY	B	192	-6.708	-0.122	9.289	1.00	10.31
7011	C	GLY	B	192	-6.208	-1.203	8.358	1.00	10.56
7012	O	GLY	B	192	-5.215	-1.020	7.668	1.00	10.85
7013	N	PHE	B	193	-6.923	-2.321	8.300	1.00	9.70
7015	CA	PHE	B	193	-6.484	-3.443	7.490	1.00	9.67
7017	CB	PHE	B	193	-7.295	-4.700	7.780	1.00	9.24
7020	CG	PHE	B	193	-6.740	-5.916	7.118	1.00	9.60
7021	CD1	PHE	B	193	-7.239	-6.357	5.893	1.00	11.05
7023	CE1	PHE	B	193	-6.695	-7.469	5.271	1.00	11.40
7025	CZ	PHE	B	193	-5.645	-8.139	5.865	1.00	11.63
7027	CE2	PHE	B	193	-5.138	-7.704	7.063	1.00	11.22
7029	CD2	PHE	B	193	-5.681	-6.599	7.690	1.00	10.48
7031	C	PHE	B	193	-6.551	-3.148	5.992	1.00	9.36
7032	O	PHE	B	193	-5.561	-3.303	5.262	1.00	9.24
7033	N	PHE	B	194	-7.733	-2.794	5.510	1.00	9.11
7035	CA	PHE	B	194	-7.931	-2.616	4.074	1.00	9.13
7037	CB	PHE	B	194	-9.418	-2.649	3.712	1.00	9.54
7040	CG	PHE	B	194	-9.976	-4.038	3.726	1.00	9.84
7041	CD1	PHE	B	194	-10.542	-4.562	4.878	1.00	9.76
7043	CE1	PHE	B	194	-11.018	-5.872	4.890	1.00	10.82
7045	CZ	PHE	B	194	-10.895	-6.663	3.766	1.00	11.13
7047	CE2	PHE	B	194	-10.312	-6.154	2.625	1.00	12.24
7049	CD2	PHE	B	194	-9.838	-4.858	2.616	1.00	11.28
7051	C	PHE	B	194	-7.214	-1.397	3.508	1.00	9.90
7052	O	PHE	B	194	-6.800	-1.421	2.351	1.00	9.84
7053	N	SER	B	195	-7.059	-0.341	4.301	1.00	9.93
7055	CA	SER	B	195	-6.256	0.801	3.867	1.00	10.52

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
7057	CB	SER	B	195	-6.444	1.997	4.789	1.00	10.59
7060	OG	SER	B	195	-7.804	2.384	4.784	1.00	10.33
7062	C	SER	B	195	-4.787	0.431	3.757	1.00	10.42
7063	O	SER	B	195	-4.088	0.955	2.902	1.00	10.61
7064	N	SER	B	196	-4.311	-0.460	4.628	1.00	9.86
7066	CA	SER	B	196	-2.935	-0.952	4.566	1.00	10.09
7068	CB	BSER	B	196	-2.584	-1.731	5.834	0.35	10.28
7069	CB	ASER	B	196	-2.565	-1.771	5.809	0.65	10.07
7074	OG	BSER	B	196	-2.265	-0.836	6.880	0.35	12.07
7075	OG	ASER	B	196	-1.287	-2.387	5.642	0.65	8.68
7078	C	SER	B	196	-2.736	-1.816	3.336	1.00	9.89
7079	O	SER	B	196	-1.767	-1.647	2.617	1.00	10.28
7080	N	ILE	B	197	-3.655	-2.753	3.086	1.00	9.77
7082	CA	ILE	B	197	-3.527	-3.592	1.903	1.00	10.76
7084	CB	BILE	B	197	-4.697	-4.632	1.902	0.35	10.20
7085	CB	AILE	B	197	-4.335	-4.923	1.915	0.65	11.84
7088	CG1	BILE	B	197	-4.608	-5.587	3.097	0.35	9.52
7089	CG1	AILE	B	197	-5.831	-4.730	1.986	0.65	13.67
7094	CD1	BILE	B	197	-3.445	-6.572	3.017	0.35	8.96
7095	CD1	AILE	B	197	-6.584	-5.960	1.472	0.65	14.81
7102	CG2	BILE	B	197	-4.762	-5.399	0.589	0.35	8.96
7103	CG2	AILE	B	197	-3.835	-5.842	3.060	0.65	12.75
7110	C	ILE	B	197	-3.636	-2.767	0.616	1.00	10.72
7111	O	ILE	B	197	-2.950	-3.079	-0.347	1.00	11.23
7112	N	ARG	B	198	-4.437	-1.701	0.601	1.00	11.00
7114	CA	ARG	B	198	-4.497	-0.857	-0.584	1.00	11.27
7116	CB	ARG	B	198	-5.489	0.291	-0.411	1.00	11.44
7119	CG	ARG	B	198	-5.691	1.087	-1.697	1.00	12.03
7122	CD	ARG	B	198	-6.503	2.344	-1.531	1.00	12.79
7125	NE	ARG	B	198	-7.891	2.097	-1.143	1.00	13.14
7127	CZ	ARG	B	198	-8.430	2.422	0.034	1.00	13.41
7128	NH1	ARG	B	198	-7.696	2.948	1.005	1.00	14.44
7131	NH2	ARG	B	198	-9.718	2.210	0.254	1.00	13.48
7134	C	ARG	B	198	-3.109	-0.306	-0.910	1.00	11.51
7135	O	ARG	B	198	-2.693	-0.293	-2.070	1.00	11.80
7136	N	LYS	B	199	-2.392	0.132	0.120	1.00	11.68
7138	CA	LYS	B	199	-1.028	0.622	-0.056	1.00	11.98
7140	CB	LYS	B	199	-0.539	1.293	1.222	1.00	12.64
7143	CG	LYS	B	199	-1.269	2.613	1.442	1.00	13.65
7146	CD	LYS	B	199	-0.943	3.257	2.741	1.00	16.59
7149	CE	LYS	B	199	-1.843	4.455	2.955	1.00	16.60
7152	NZ	LYS	B	199	-1.851	5.467	1.862	1.00	17.18
7156	C	LYS	B	199	-0.079	-0.479	-0.530	1.00	11.97
7157	O	LYS	B	199	0.770	-0.246	-1.375	1.00	12.47
7158	N	GLU	B	200	-0.258	-1.689	-0.015	1.00	11.75
7160	CA	GLU	B	200	0.550	-2.821	-0.447	1.00	11.92
7162	CB	GLU	B	200	0.275	-4.041	0.430	1.00	11.83
7165	CG	GLU	B	200	0.717	-3.805	1.862	1.00	11.98
7168	CD	GLU	B	200	0.612	-5.024	2.756	1.00	13.26

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
7169	OE1	GLU	B	200	0.872	-4.850	3.967	1.00	13.29
7170	OE2	GLU	B	200	0.261	-6.129	2.280	1.00	11.54
7171	C	GLU	B	200	0.286	-3.159	-1.898	1.00	12.45
7172	O	GLU	B	200	1.205	-3.514	-2.613	1.00	13.09
7173	N	TYR	B	201	-0.969	-3.080	-2.337	1.00	12.52
7175	CA	TYR	B	201	-1.283	-3.370	-3.734	1.00	13.50
7177	CB	TYR	B	201	-2.788	-3.450	-3.998	1.00	12.95
7180	CG	TYR	B	201	-3.491	-4.638	-3.373	1.00	13.96
7181	CD1	TYR	B	201	-2.784	-5.624	-2.680	1.00	15.84
7183	CE1	TYR	B	201	-3.443	-6.706	-2.107	1.00	17.27
7185	CZ	TYR	B	201	-4.807	-6.811	-2.227	1.00	18.05
7186	OH	TYR	B	201	-5.480	-7.865	-1.653	1.00	23.09
7188	CE2	TYR	B	201	-5.529	-5.859	-2.912	1.00	16.69
7190	CD2	TYR	B	201	-4.871	-4.779	-3.488	1.00	14.83
7192	C	TYR	B	201	-0.653	-2.327	-4.643	1.00	14.54
7193	O	TYR	B	201	-0.263	-2.651	-5.758	1.00	14.82
7194	N	SER	B	202	-0.541	-1.084	-4.176	1.00	15.83
7196	CA	SER	B	202	0.124	-0.047	-4.977	1.00	17.14
7198	CB	BSER	B	202	-0.048	1.333	-4.337	0.35	17.06
7199	CB	ASER	B	202	-0.038	1.329	-4.331	0.65	17.29
7204	OG	BSER	B	202	0.618	2.332	-5.093	0.35	16.87
7205	OG	ASER	B	202	-1.398	1.621	-4.078	0.65	18.68
7208	C	SER	B	202	1.607	-0.361	-5.184	1.00	17.90
7209	O	SER	B	202	2.108	-0.259	-6.309	1.00	18.61
7210	N	VAL	B	203	2.311	-0.760	-4.120	1.00	18.56
7212	CA	VAL	B	203	3.750	-1.047	-4.246	1.00	18.86
7214	CB	BVAL	B	203	4.527	-0.999	-2.873	0.35	19.08
7215	CB	AVAL	B	203	4.505	-0.939	-2.892	0.65	19.42
7218	CG1	BVAL	B	203	3.900	-0.011	-1.893	0.35	18.74
7219	CG1	AVAL	B	203	4.543	0.511	-2.431	0.65	19.82
7226	CG2	BVAL	B	203	4.655	-2.386	-2.231	0.35	19.17
7227	CG2	AVAL	B	203	3.887	-1.817	-1.832	0.65	19.25
7234	C	VAL	B	203	4.019	-2.386	-4.952	1.00	18.83
7235	O	VAL	B	203	5.032	-2.517	-5.642	1.00	19.05
7236	N	SER	B	204	3.115	-3.357	-4.804	1.00	17.91
7238	CA	SER	B	204	3.263	-4.669	-5.443	1.00	17.77
7240	CB	BSER	B	204	2.727	-5.793	-4.544	0.35	17.81
7241	CB	ASER	B	204	2.627	-5.770	-4.586	0.65	18.25
7246	OG	BSER	B	204	1.379	-5.583	-4.171	0.35	17.15
7247	OG	ASER	B	204	3.309	-5.945	-3.366	0.65	20.23
7250	C	SER	B	204	2.613	-4.708	-6.835	1.00	17.20
7251	O	SER	B	204	2.649	-5.737	-7.495	1.00	16.75
7252	N	ARG	B	205	2.023	-3.594	-7.269	1.00	16.27
7254	CA	ARG	B	205	1.372	-3.502	-8.585	1.00	16.65
7256	CB	ARG	B	205	2.426	-3.524	-9.697	1.00	17.54
7259	CG	ARG	B	205	3.446	-2.426	-9.518	1.00	20.28
7262	CD	ARG	B	205	4.084	-1.945	-10.808	1.00	24.36
7265	NE	ARG	B	205	5.080	-2.895	-11.297	1.00	27.85
7267	CZ	ARG	B	205	6.201	-2.570	-11.950	1.00	30.37

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
7268	NH1	ARG	B	205	6.503	-1.299	-12.217	1.00	31.90
7271	NH2	ARG	B	205	7.033	-3.529	-12.343	1.00	32.06
7274	C	ARG	B	205	0.280	-4.549	-8.800	1.00	16.17
7275	O	ARG	B	205	0.195	-5.208	-9.842	1.00	16.15
7276	N	VAL	B	206	-0.561	-4.695	-7.787	1.00	14.89
7278	CA	VAL	B	206	-1.745	-5.534	-7.880	1.00	14.33
7280	CB	VAL	B	206	-2.058	-6.212	-6.538	1.00	14.18
7282	CG1	VAL	B	206	-3.390	-6.954	-6.601	1.00	14.04
7286	CG2	VAL	B	206	-0.930	-7.167	-6.146	1.00	13.98
7290	C	VAL	B	206	-2.903	-4.639	-8.303	1.00	14.42
7291	O	VAL	B	206	-3.248	-3.693	-7.597	1.00	14.75
7292	N	ASN	B	207	-3.510	-4.953	-9.446	1.00	14.06
7294	CA	ASN	B	207	-4.534	-4.103	-10.049	1.00	14.20
7296	CB	ASN	B	207	-4.430	-4.165	-11.585	1.00	14.73
7299	CG	ASN	B	207	-5.192	-3.038	-12.270	1.00	17.92
7300	OD1	ASN	B	207	-5.525	-2.028	-11.641	1.00	22.61
7301	ND2	ASN	B	207	-5.457	-3.198	-13.565	1.00	21.33
7304	C	ASN	B	207	-5.943	-4.488	-9.586	1.00	13.25
7305	O	ASN	B	207	-6.827	-4.775	-10.393	1.00	13.76
7306	N	VAL	B	208	-6.124	-4.498	-8.266	1.00	12.11
7308	CA	VAL	B	208	-7.402	-4.762	-7.622	1.00	11.71
7310	CB	VAL	B	208	-7.328	-6.036	-6.763	1.00	11.42
7312	CG1	VAL	B	208	-8.621	-6.226	-5.916	1.00	12.16
7316	CG2	VAL	B	208	-7.055	-7.259	-7.638	1.00	12.23
7320	C	VAL	B	208	-7.721	-3.550	-6.751	1.00	11.16
7321	O	VAL	B	208	-6.914	-3.163	-5.902	1.00	11.33
7322	N	SER	B	209	-8.866	-2.923	-6.990	1.00	10.70
7324	CA	SER	B	209	-9.242	-1.720	-6.247	1.00	10.48
7326	CB	SER	B	209	-10.145	-0.814	-7.077	1.00	10.69
7329	OG	SER	B	209	-11.373	-1.440	-7.399	1.00	11.75
7331	C	SER	B	209	-9.908	-2.093	-4.922	1.00	10.01
7332	O	SER	B	209	-10.499	-3.157	-4.798	1.00	9.89
7333	N	ILE	B	210	-9.767	-1.210	-3.944	1.00	10.03
7335	CA	ILE	B	210	-10.419	-1.331	-2.644	1.00	10.61
7337	CB	ILE	B	210	-9.390	-1.631	-1.525	1.00	10.69
7339	CG1	ILE	B	210	-8.725	-2.994	-1.744	1.00	11.41
7342	CD1	ILE	B	210	-7.526	-3.250	-0.867	1.00	12.15
7346	CG2	ILE	B	210	-10.058	-1.610	-0.156	1.00	11.69
7350	C	ILE	B	210	-11.162	-0.028	-2.354	1.00	10.96
7351	O	ILE	B	210	-10.561	1.049	-2.341	1.00	10.99
7352	N	THR	B	211	-12.466	-0.139	-2.109	1.00	11.44
7354	CA	THR	B	211	-13.334	0.992	-1.831	1.00	11.79
7356	CB	THR	B	211	-14.484	1.016	-2.853	1.00	11.55
7358	OG1	THR	B	211	-13.961	1.133	-4.192	1.00	12.06
7360	CG2	THR	B	211	-15.353	2.230	-2.670	1.00	11.79
7364	C	THR	B	211	-13.910	0.802	-0.447	1.00	11.64
7365	O	THR	B	211	-14.583	-0.203	-0.206	1.00	12.36
7366	N	LEU	B	212	-13.650	1.739	0.453	1.00	11.05
7368	CA	LEU	B	212	-14.239	1.733	1.789	1.00	11.17

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
7370	CB	LEU	B	212	-13.198	2.137	2.835	1.00	11.04
7373	CG	LEU	B	212	-13.637	2.124	4.308	1.00	11.93
7375	CD1	LEU	B	212	-12.576	2.789	5.160	1.00	14.69
7379	CD2	LEU	B	212	-13.886	0.711	4.774	1.00	13.42
7383	C	LEU	B	212	-15.409	2.702	1.824	1.00	11.32
7384	O	LEU	B	212	-15.252	3.866	1.471	1.00	12.08
7385	N	CYS	B	213	-16.576	2.228	2.264	1.00	11.29
7387	CA	CYS	B	213	-17.805	3.022	2.259	1.00	11.65
7389	CB	CYS	B	213	-18.952	2.188	1.707	1.00	12.12
7392	SG	CYS	B	213	-18.577	1.572	0.069	1.00	15.40
7393	C	CYS	B	213	-18.097	3.442	3.678	1.00	11.82
7394	O	CYS	B	213	-17.989	2.632	4.591	1.00	13.43
7395	N	VAL	B	214	-18.416	4.709	3.882	1.00	10.75
7397	CA	VAL	B	214	-18.670	5.237	5.220	1.00	10.92
7399	CB	VAL	B	214	-17.675	6.364	5.546	1.00	10.83
7401	CG1	VAL	B	214	-18.003	7.019	6.892	1.00	12.07
7405	CG2	VAL	B	214	-16.254	5.835	5.548	1.00	12.08
7409	C	VAL	B	214	-20.098	5.766	5.251	1.00	10.89
7410	O	VAL	B	214	-20.418	6.762	4.590	1.00	11.66
7411	N	LEU	B	215	-20.965	5.081	5.990	1.00	10.35
7413	CA	LEU	B	215	-22.406	5.356	5.946	1.00	10.42
7415	CB	LEU	B	215	-23.176	4.058	5.697	1.00	10.13
7418	CG	LEU	B	215	-22.726	3.218	4.497	1.00	10.67
7420	CD1	LEU	B	215	-23.642	2.025	4.347	1.00	11.48
7424	CD2	LEU	B	215	-22.626	4.010	3.204	1.00	12.21
7428	C	LEU	B	215	-22.945	5.997	7.201	1.00	9.79
7429	O	LEU	B	215	-22.640	5.575	8.309	1.00	10.80
7430	N	GLY	B	216	-23.798	7.001	7.019	1.00	10.34
7432	CA	GLY	B	216	-24.593	7.546	8.102	1.00	10.49
7435	C	GLY	B	216	-25.844	6.719	8.304	1.00	10.54
7436	O	GLY	B	216	-25.877	5.530	7.967	1.00	11.01
7437	N	LEU	B	217	-26.870	7.336	8.872	1.00	10.50
7439	CA	LEU	B	217	-28.108	6.619	9.158	1.00	10.52
7441	CB	LEU	B	217	-28.999	7.438	10.098	1.00	10.86
7444	CG	LEU	B	217	-30.328	6.795	10.519	1.00	11.32
7446	CD1	LEU	B	217	-30.094	5.482	11.240	1.00	11.10
7450	CD2	LEU	B	217	-31.134	7.748	11.389	1.00	11.10
7454	C	LEU	B	217	-28.860	6.300	7.868	1.00	10.61
7455	O	LEU	B	217	-29.216	7.201	7.117	1.00	10.95
7456	N	ILE	B	218	-29.119	5.015	7.651	1.00	10.23
7458	CA	ILE	B	218	-29.802	4.516	6.460	1.00	10.15
7460	CB	ILE	B	218	-28.908	3.508	5.674	1.00	10.76
7462	CG1	ILE	B	218	-27.460	4.007	5.535	1.00	10.83
7465	CD1	ILE	B	218	-27.284	5.362	4.823	1.00	12.05
7469	CG2	ILE	B	218	-29.521	3.200	4.305	1.00	10.95
7473	C	ILE	B	218	-31.056	3.796	6.931	1.00	10.66
7474	O	ILE	B	218	-31.014	3.060	7.911	1.00	10.02
7475	N	ASP	B	219	-32.156	3.984	6.213	1.00	10.31
7477	CA	ASP	B	219	-33.483	3.516	6.665	1.00	10.38

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
7479	CB	ASP	B	219	-34.583	4.320	5.956	1.00	10.41
7482	CG	ASP	B	219	-34.662	4.043	4.478	1.00	11.92
7483	OD1	ASP	B	219	-35.546	4.640	3.808	1.00	13.77
7484	OD2	ASP	B	219	-33.900	3.237	3.885	1.00	11.88
7485	C	ASP	B	219	-33.765	2.007	6.543	1.00	10.34
7486	O	ASP	B	219	-34.900	1.594	6.264	1.00	10.76
7487	N	THR	B	220	-32.752	1.175	6.769	1.00	10.14
7489	CA	THR	B	220	-32.982	-0.268	6.839	1.00	9.80
7491	CB	THR	B	220	-31.648	-1.052	6.884	1.00	9.33
7493	OG1	THR	B	220	-30.935	-0.774	8.097	1.00	10.11
7495	CG2	THR	B	220	-30.720	-0.670	5.743	1.00	10.26
7499	C	THR	B	220	-33.815	-0.615	8.063	1.00	9.87
7500	O	THR	B	220	-33.816	0.111	9.049	1.00	9.67
7501	N	GLU	B	221	-34.526	-1.738	8.007	1.00	10.11
7503	CA	GLU	B	221	-35.305	-2.168	9.161	1.00	11.25
7505	CB	GLU	B	221	-36.022	-3.482	8.869	1.00	11.92
7508	CG	GLU	B	221	-37.062	-3.401	7.768	1.00	13.84
7511	CD	GLU	B	221	-38.004	-2.217	7.918	1.00	17.41
7512	OE1	GLU	B	221	-38.028	-1.383	6.994	1.00	20.81
7513	OE2	GLU	B	221	-38.718	-2.129	8.945	1.00	18.79
7514	C	GLU	B	221	-34.436	-2.293	10.412	1.00	10.67
7515	O	GLU	B	221	-34.815	-1.874	11.479	1.00	10.38
7516	N	THR	B	222	-33.240	-2.845	10.274	1.00	10.92
7518	CA	THR	B	222	-32.344	-2.988	11.411	1.00	11.04
7520	CB	THR	B	222	-31.051	-3.638	10.938	1.00	11.25
7522	OG1	THR	B	222	-31.319	-5.005	10.606	1.00	10.97
7524	CG2	THR	B	222	-29.996	-3.661	12.043	1.00	11.76
7528	C	THR	B	222	-32.052	-1.646	12.076	1.00	10.99
7529	O	THR	B	222	-32.153	-1.509	13.283	1.00	11.01
7530	N	ALA	B	223	-31.691	-0.651	11.268	1.00	10.76
7532	CA	ALA	B	223	-31.325	0.646	11.807	1.00	10.99
7534	CB	ALA	B	223	-30.714	1.517	10.728	1.00	10.70
7538	C	ALA	B	223	-32.530	1.335	12.426	1.00	10.95
7539	O	ALA	B	223	-32.433	1.917	13.494	1.00	11.55
7540	N	MET	B	224	-33.670	1.236	11.759	1.00	11.07
7542	CA	MET	B	224	-34.856	1.963	12.187	1.00	11.99
7544	CB	MET	B	224	-35.893	1.928	11.074	1.00	11.67
7547	CG	MET	B	224	-35.448	2.641	9.795	1.00	12.08
7550	SD	MET	B	224	-35.230	4.426	10.001	1.00	14.55
7551	CE	MET	B	224	-33.504	4.544	10.420	1.00	13.47
7555	C	MET	B	224	-35.377	1.406	13.507	1.00	12.29
7556	O	MET	B	224	-35.805	2.164	14.387	1.00	12.73
7557	N	LYS	B	225	-35.306	0.083	13.672	1.00	12.69
7559	CA	LYS	B	225	-35.637	-0.546	14.948	1.00	13.43
7561	CB	LYS	B	225	-35.691	-2.075	14.807	1.00	13.90
7564	CG	LYS	B	225	-36.898	-2.604	14.075	1.00	17.24
7567	CD	LYS	B	225	-36.872	-4.139	14.104	1.00	20.63
7570	CE	LYS	B	225	-38.089	-4.779	13.501	1.00	24.77
7573	NZ	LYS	B	225	-37.768	-5.669	12.332	1.00	26.89

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
7577	C	LYS	B	225	-34.637	-0.171	16.042	1.00	13.77
7578	O	LYS	B	225	-35.011	0.112	17.183	1.00	14.16
7579	N	ALA	B	226	-33.357	-0.155	15.688	1.00	13.62
7581	CA	ALA	B	226	-32.300	0.051	16.662	1.00	14.17
7583	CB	ALA	B	226	-30.944	-0.234	16.017	1.00	14.38
7587	C	ALA	B	226	-32.302	1.443	17.270	1.00	14.61
7588	O	ALA	B	226	-32.004	1.601	18.451	1.00	14.97
7589	N	VAL	B	227	-32.655	2.449	16.480	1.00	14.63
7591	CA	VAL	B	227	-32.522	3.830	16.922	1.00	15.33
7593	CB	VAL	B	227	-31.989	4.748	15.796	1.00	15.02
7595	CG1	VAL	B	227	-30.652	4.244	15.283	1.00	14.46
7599	CG2	VAL	B	227	-32.993	4.920	14.659	1.00	14.68
7603	C	VAL	B	227	-33.821	4.399	17.474	1.00	16.76
7604	O	VAL	B	227	-33.840	5.525	17.955	1.00	17.18
7605	N	SER	B	228	-34.887	3.603	17.406	1.00	18.11
7607	CA	SER	B	228	-36.210	4.006	17.882	1.00	19.66
7609	CB	SER	B	228	-37.165	2.813	17.783	1.00	19.87
7612	OG	SER	B	228	-38.378	3.064	18.459	1.00	21.76
7614	C	SER	B	228	-36.140	4.514	19.317	1.00	20.25
7615	O	SER	B	228	-35.707	3.790	20.219	1.00	21.00
7616	N	GLY	B	229	-36.527	5.773	19.512	1.00	21.33
7618	CA	GLY	B	229	-36.507	6.409	20.823	1.00	21.68
7621	C	GLY	B	229	-35.190	7.041	21.245	1.00	22.30
7622	O	GLY	B	229	-35.160	7.824	22.194	1.00	22.20
7623	N	ILE	B	230	-34.104	6.707	20.551	1.00	22.47
7625	CA	ILE	B	230	-32.766	7.217	20.874	1.00	23.46
7627	CB	ILE	B	230	-31.690	6.120	20.659	1.00	23.53
7629	CG1	ILE	B	230	-32.110	4.787	21.277	1.00	25.04
7632	CD1	ILE	B	230	-32.563	4.885	22.700	1.00	26.14
7636	CG2	ILE	B	230	-30.335	6.591	21.199	1.00	23.50
7640	C	ILE	B	230	-32.388	8.400	20.000	1.00	23.86
7641	O	ILE	B	230	-31.793	9.370	20.464	1.00	23.99
7642	N	VAL	B	231	-32.705	8.289	18.719	1.00	24.75
7644	CA	VAL	B	231	-32.311	9.267	17.728	1.00	25.51
7646	CB	VAL	B	231	-31.362	8.607	16.708	1.00	26.00
7648	CG1	VAL	B	231	-31.216	9.438	15.465	1.00	27.56
7652	CG2	VAL	B	231	-30.011	8.347	17.350	1.00	26.14
7656	C	VAL	B	231	-33.534	9.832	17.013	1.00	25.49
7657	O	VAL	B	231	-34.522	9.134	16.776	1.00	25.73
7658	N	HIS	B	232	-33.456	11.117	16.698	1.00	25.39
7660	CA	HIS	B	232	-34.427	11.791	15.858	1.00	25.54
7662	CB	HIS	B	232	-35.320	12.708	16.692	1.00	26.04
7665	CG	HIS	B	232	-36.147	11.989	17.707	1.00	28.51
7666	ND1	HIS	B	232	-36.130	12.318	19.046	1.00	31.50
7668	CE1	HIS	B	232	-36.961	11.527	19.701	1.00	32.45
7670	NE2	HIS	B	232	-37.518	10.698	18.836	1.00	32.18
7672	CD2	HIS	B	232	-37.028	10.969	17.581	1.00	31.04
7674	C	HIS	B	232	-33.633	12.600	14.840	1.00	24.42
7675	O	HIS	B	232	-33.300	13.760	15.068	1.00	25.65



# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
7676	N	MET	B	233	-33.254	11.945	13.752	1.00	22.60
7678	CA	MET	B	233	-32.650	12.628	12.611	1.00	20.79
7680	CB	MET	B	233	-31.120	12.612	12.706	1.00	20.37
7683	CG	MET	B	233	-30.513	11.236	12.626	1.00	19.21
7686	SD	MET	B	233	-28.739	11.251	12.892	1.00	18.15
7687	CE	MET	B	233	-28.637	11.470	14.653	1.00	16.65
7691	C	MET	B	233	-33.129	11.980	11.319	1.00	19.81
7692	O	MET	B	233	-33.839	10.976	11.343	1.00	19.44
7693	N	GLN	B	234	-32.766	12.570	10.188	1.00	18.67
7695	CA	GLN	B	234	-33.193	12.041	8.899	1.00	18.42
7697	CB	GLN	B	234	-32.908	13.034	7.777	1.00	19.13
7700	CG	GLN	B	234	-33.747	14.303	7.857	1.00	22.36
7703	CD	GLN	B	234	-35.212	14.057	7.545	1.00	26.30
7704	OE1	GLN	B	234	-36.083	14.285	8.392	1.00	30.03
7705	NE2	GLN	B	234	-35.490	13.584	6.335	1.00	29.20
7708	C	GLN	B	234	-32.479	10.729	8.623	1.00	17.16
7709	O	GLN	B	234	-31.328	10.559	8.989	1.00	16.54
7710	N	ALA	B	235	-33.184	9.791	8.006	1.00	15.84
7712	CA	ALA	B	235	-32.563	8.553	7.546	1.00	15.29
7714	CB	ALA	B	235	-33.332	7.370	8.066	1.00	14.89
7718	C	ALA	B	235	-32.551	8.554	6.026	1.00	14.93
7719	O	ALA	B	235	-33.580	8.845	5.392	1.00	15.91
7720	N	ALA	B	236	-31.402	8.230	5.438	1.00	13.69
7722	CA	ALA	B	236	-31.253	8.205	3.984	1.00	13.16
7724	CB	ALA	B	236	-29.796	8.314	3.612	1.00	12.83
7728	C	ALA	B	236	-31.862	6.934	3.390	1.00	13.10
7729	O	ALA	B	236	-31.887	5.890	4.048	1.00	13.11
7730	N	PRO	B	237	-32.341	7.007	2.155	1.00	12.79
7731	CA	PRO	B	237	-32.955	5.839	1.516	1.00	12.55
7733	CB	PRO	B	237	-33.619	6.412	0.255	1.00	13.14
7736	CG	PRO	B	237	-32.968	7.715	0.010	1.00	13.89
7739	CD	PRO	B	237	-32.363	8.200	1.289	1.00	13.35
7742	C	PRO	B	237	-31.936	4.750	1.169	1.00	12.24
7743	O	PRO	B	237	-30.916	5.002	0.525	1.00	12.31
7744	N	LYS	B	238	-32.241	3.535	1.596	1.00	11.92
7746	CA	LYS	B	238	-31.364	2.391	1.386	1.00	12.01
7748	CB	LYS	B	238	-31.930	1.153	2.096	1.00	11.80
7751	CG	LYS	B	238	-33.354	0.767	1.716	1.00	12.22
7754	CD	LYS	B	238	-33.823	-0.377	2.569	1.00	13.37
7757	CE	LYS	B	238	-35.179	-0.898	2.108	1.00	13.68
7760	NZ	LYS	B	238	-35.716	-1.960	3.028	1.00	14.84
7764	C	LYS	B	238	-31.110	2.090	-0.094	1.00	12.18
7765	O	LYS	B	238	-30.037	1.618	-0.466	1.00	12.12
7766	N	GLU	B	239	-32.098	2.361	-0.939	1.00	12.75
7768	CA	GLU	B	239	-31.968	2.139	-2.369	1.00	13.85
7770	CB	GLU	B	239	-33.316	2.389	-3.053	1.00	14.87
7773	CG	GLU	B	239	-34.424	1.440	-2.595	1.00	17.43
7776	CD	GLU	B	239	-35.236	1.905	-1.372	1.00	20.25
7777	OE1	GLU	B	239	-34.949	2.982	-0.759	1.00	17.06

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
7778	OE2	GLU	B	239	-36.195	1.154	-1.022	1.00	23.38
7779	C	GLU	B	239	-30.883	3.046	-2.956	1.00	13.21
7780	O	GLU	B	239	-30.034	2.593	-3.722	1.00	12.93
7781	N	GLU	B	240	-30.897	4.318	-2.569	1.00	13.33
7783	CA	GLU	B	240	-29.906	5.280	-3.064	1.00	13.65
7785	CB	GLU	B	240	-30.299	6.712	-2.721	1.00	14.49
7788	CG	GLU	B	240	-29.317	7.738	-3.263	1.00	18.44
7791	CD	GLU	B	240	-29.781	9.168	-3.067	1.00	22.98
7792	OE1	GLU	B	240	-30.281	9.775	-4.047	1.00	29.75
7793	OE2	GLU	B	240	-29.650	9.693	-1.942	1.00	24.99
7794	C	GLU	B	240	-28.531	4.967	-2.487	1.00	12.54
7795	O	GLU	B	240	-27.527	5.048	-3.192	1.00	11.92
7796	N	CYS	B	241	-28.496	4.593	-1.214	1.00	11.78
7798	CA	CYS	B	241	-27.248	4.217	-0.552	1.00	11.84
7800	CB	CYS	B	241	-27.530	3.771	0.876	1.00	11.72
7803	SG	CYS	B	241	-26.079	3.283	1.817	1.00	13.87
7804	C	CYS	B	241	-26.551	3.096	-1.318	1.00	11.36
7805	O	CYS	B	241	-25.362	3.178	-1.618	1.00	12.56
7806	N	ALA	B	242	-27.309	2.043	-1.613	1.00	11.13
7808	CA	ALA	B	242	-26.800	0.881	-2.325	1.00	11.03
7810	CB	ALA	B	242	-27.915	-0.140	-2.495	1.00	11.07
7814	C	ALA	B	242	-26.237	1.269	-3.688	1.00	11.62
7815	O	ALA	B	242	-25.198	0.755	-4.099	1.00	12.12
7816	N	LEU	B	243	-26.919	2.171	-4.392	1.00	11.85
7818	CA	LEU	B	243	-26.452	2.574	-5.714	1.00	12.49
7820	CB	LEU	B	243	-27.499	3.396	-6.455	1.00	12.70
7823	CG	LEU	B	243	-27.135	3.809	-7.886	1.00	13.71
7825	CD1	LEU	B	243	-26.846	2.596	-8.752	1.00	15.54
7829	CD2	LEU	B	243	-28.262	4.634	-8.468	1.00	16.34
7833	C	LEU	B	243	-25.146	3.355	-5.612	1.00	12.60
7834	O	LEU	B	243	-24.238	3.138	-6.408	1.00	13.22
7835	N	GLU	B	244	-25.026	4.238	-4.629	1.00	13.13
7837	CA	GLU	B	244	-23.783	5.002	-4.472	1.00	13.43
7839	CB	GLU	B	244	-23.949	6.121	-3.437	1.00	13.78
7842	CG	GLU	B	244	-24.878	7.250	-3.863	1.00	16.59
7845	CD	GLU	B	244	-24.495	7.916	-5.182	1.00	20.36
7846	OE1	GLU	B	244	-25.411	8.279	-5.948	1.00	23.95
7847	OE2	GLU	B	244	-23.290	8.085	-5.456	1.00	22.51
7848	C	GLU	B	244	-22.590	4.108	-4.112	1.00	13.06
7849	O	GLU	B	244	-21.463	4.371	-4.526	1.00	13.45
7850	N	ILE	B	245	-22.839	3.030	-3.375	1.00	12.16
7852	CA	ILE	B	245	-21.787	2.069	-3.064	1.00	12.01
7854	CB	ILE	B	245	-22.265	1.037	-2.018	1.00	11.84
7856	CG1	ILE	B	245	-22.450	1.733	-0.655	1.00	12.13
7859	CD1	ILE	B	245	-23.201	0.894	0.379	1.00	12.63
7863	CG2	ILE	B	245	-21.289	-0.153	-1.940	1.00	11.58
7867	C	ILE	B	245	-21.313	1.375	-4.340	1.00	12.44
7868	O	ILE	B	245	-20.115	1.281	-4.578	1.00	11.98
7869	N	ILE	B	246	-22.253	0.884	-5.150	1.00	12.81

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
7871	CA	ILE	B	246	-21.908	0.231	-6.420	1.00	12.90
7873	CB	ILE	B	246	-23.163	-0.309	-7.120	1.00	12.91
7875	CG1	ILE	B	246	-23.754	-1.460	-6.290	1.00	12.60
7878	CD1	ILE	B	246	-25.192	-1.745	-6.606	1.00	13.67
7882	CG2	ILE	B	246	-22.836	-0.776	-8.545	1.00	13.68
7886	C	ILE	B	246	-21.148	1.181	-7.343	1.00	13.52
7887	O	ILE	B	246	-20.140	0.791	-7.927	1.00	13.62
7888	N	LYS	B	247	-21.625	2.416	-7.468	1.00	14.06
7890	CA	LYS	B	247	-20.970	3.405	-8.326	1.00	14.69
7892	CB	LYS	B	247	-21.711	4.747	-8.294	1.00	15.04
7895	CG	LYS	B	247	-23.047	4.752	-8.988	1.00	18.01
7898	CD	LYS	B	247	-23.706	6.116	-8.871	1.00	22.58
7901	CE	LYS	B	247	-24.882	6.269	-9.818	1.00	25.17
7904	NZ	LYS	B	247	-25.505	7.616	-9.665	1.00	27.36
7908	C	LYS	B	247	-19.529	3.624	-7.885	1.00	14.43
7909	O	LYS	B	247	-18.623	3.653	-8.713	1.00	14.95
7910	N	GLY	B	248	-19.322	3.790	-6.585	1.00	14.40
7912	CA	GLY	B	248	-17.991	4.001	-6.049	1.00	14.38
7915	C	GLY	B	248	-17.059	2.834	-6.327	1.00	14.08
7916	O	GLY	B	248	-15.911	3.034	-6.692	1.00	14.30
7917	N	GLY	B	249	-17.554	1.612	-6.167	1.00	14.32
7919	CA	GLY	B	249	-16.776	0.423	-6.456	1.00	13.50
7922	C	GLY	B	249	-16.446	0.292	-7.936	1.00	13.82
7923	O	GLY	B	249	-15.315	-0.032	-8.297	1.00	14.64
7924	N	ALA	B	250	-17.438	0.551	-8.781	1.00	13.68
7926	CA	ALA	B	250	-17.290	0.469	-10.229	1.00	13.73
7928	CB	ALA	B	250	-18.622	0.701	-10.900	1.00	14.09
7932	C	ALA	B	250	-16.268	1.479	-10.733	1.00	13.57
7933	O	ALA	B	250	-15.508	1.193	-11.669	1.00	14.50
7934	N	LEU	B	251	-16.241	2.652	-10.106	1.00	12.96
7936	CA	LEU	B	251	-15.302	3.713	-10.482	1.00	12.56
7938	CB	LEU	B	251	-15.924	5.087	-10.235	1.00	12.83
7941	CG	LEU	B	251	-17.179	5.400	-11.053	1.00	13.10
7943	CD1	LEU	B	251	-17.735	6.738	-10.624	1.00	13.88
7947	CD2	LEU	B	251	-16.877	5.383	-12.549	1.00	13.61
7951	C	LEU	B	251	-13.966	3.609	-9.746	1.00	12.78
7952	O	LEU	B	251	-13.102	4.476	-9.902	1.00	12.57
7953	N	ARG	B	252	-13.807	2.563	-8.934	1.00	12.68
7955	CA	ARG	B	252	-12.542	2.278	-8.252	1.00	12.81
7957	CB	ARG	B	252	-11.450	1.936	-9.278	1.00	12.72
7960	CG	ARG	B	252	-11.848	0.854	-10.265	1.00	12.91
7963	CD	ARG	B	252	-10.786	0.559	-11.324	1.00	13.85
7966	NE	ARG	B	252	-9.750	-0.370	-10.865	1.00	12.37
7968	CZ	ARG	B	252	-9.898	-1.692	-10.776	1.00	13.56
7969	NH1	ARG	B	252	-11.039	-2.280	-11.103	1.00	13.88
7972	NH2	ARG	B	252	-8.877	-2.437	-10.376	1.00	14.94
7975	C	ARG	B	252	-12.095	3.411	-7.329	1.00	13.09
7976	O	ARG	B	252	-10.904	3.671	-7.160	1.00	12.90
7977	N	GLN	B	253	-13.068	4.075	-6.713	1.00	13.58

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
7979	CA	GLN	B	253	-12.800	5.125	-5.749	1.00	14.02
7981	CB	GLN	B	253	-14.078	5.916	-5.466	1.00	14.80
7984	CG	GLN	B	253	-14.597	6.721	-6.639	1.00	17.82
7987	CD	GLN	B	253	-15.978	7.300	-6.376	1.00	18.47
7988	OE1	GLN	B	253	-16.456	7.295	-5.240	1.00	25.71
7989	NE2	GLN	B	253	-16.619	7.791	-7.420	1.00	24.02
7992	C	GLN	B	253	-12.289	4.529	-4.436	1.00	14.01
7993	O	GLN	B	253	-12.682	3.425	-4.049	1.00	14.04
7994	N	GLU	B	254	-11.425	5.257	-3.741	1.00	13.56
7996	CA	GLU	B	254	-10.901	4.769	-2.467	1.00	14.26
7998	CB	GLU	B	254	-9.674	5.564	-2.024	1.00	14.78
8001	CG	GLU	B	254	-8.525	5.380	-3.004	1.00	17.36
8004	CD	GLU	B	254	-7.171	5.816	-2.476	1.00	22.30
8005	OE1	GLU	B	254	-6.212	5.795	-3.275	1.00	26.53
8006	OE2	GLU	B	254	-7.054	6.160	-1.287	1.00	25.82
8007	C	GLU	B	254	-11.963	4.770	-1.378	1.00	13.94
8008	O	GLU	B	254	-12.055	3.819	-0.618	1.00	12.66
8009	N	GLU	B	255	-12.762	5.831	-1.320	1.00	15.01
8011	CA	GLU	B	255	-13.770	5.973	-0.272	1.00	15.77
8013	CB	GLU	B	255	-13.210	6.800	0.914	1.00	16.30
8016	CG	GLU	B	255	-12.044	6.103	1.645	1.00	18.53
8019	CD	GLU	B	255	-11.679	6.677	3.029	1.00	22.66
8020	OE1	GLU	B	255	-11.018	5.969	3.839	1.00	23.75
8021	OE2	GLU	B	255	-12.019	7.834	3.316	1.00	23.84
8022	C	GLU	B	255	-15.090	6.519	-0.836	1.00	15.86
8023	O	GLU	B	255	-15.098	7.320	-1.777	1.00	17.19
8024	N	VAL	B	256	-16.194	6.001	-0.309	1.00	14.66
8026	CA	VAL	B	256	-17.542	6.496	-0.590	1.00	14.63
8028	CB	VAL	B	256	-18.456	5.394	-1.156	1.00	15.32
8030	CG1	VAL	B	256	-19.919	5.868	-1.217	1.00	16.33
8034	CG2	VAL	B	256	-17.963	4.946	-2.518	1.00	16.42
8038	C	VAL	B	256	-18.112	6.956	0.732	1.00	13.96
8039	O	VAL	B	256	-18.065	6.223	1.719	1.00	14.84
8040	N	TYR	B	257	-18.624	8.177	0.770	1.00	13.12
8042	CA	TYR	B	257	-19.294	8.707	1.948	1.00	13.09
8044	CB	TYR	B	257	-18.633	10.027	2.393	1.00	13.44
8047	CG	TYR	B	257	-17.256	9.812	2.977	1.00	13.61
8048	CD1	TYR	B	257	-16.133	9.792	2.176	1.00	17.63
8050	CE1	TYR	B	257	-14.858	9.558	2.733	1.00	17.29
8052	CZ	TYR	B	257	-14.740	9.338	4.091	1.00	18.07
8053	OH	TYR	B	257	-13.502	9.104	4.672	1.00	19.81
8055	CE2	TYR	B	257	-15.848	9.356	4.889	1.00	17.24
8057	CD2	TYR	B	257	-17.095	9.586	4.337	1.00	16.04
8059	C	TYR	B	257	-20.746	8.948	1.559	1.00	13.03
8060	O	TYR	B	257	-21.011	9.593	0.544	1.00	13.29
8061	N	TYR	B	258	-21.677	8.436	2.358	1.00	12.26
8063	CA	TYR	B	258	-23.099	8.572	2.069	1.00	12.22
8065	CB	TYR	B	258	-23.639	7.335	1.346	1.00	12.46
8068	CG	TYR	B	258	-25.074	7.518	0.952	1.00	13.55

## FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
8069	CD1	TYR	B	258	-26.098	7.040	1.751	1.00	14.03
8071	CE1	TYR	B	258	-27.416	7.232	1.418	1.00	15.60
8073	CZ	TYR	B	258	-27.738	7.934	0.280	1.00	15.83
8074	OH	TYR	B	258	-29.057	8.150	-0.046	1.00	19.89
8076	CE2	TYR	B	258	-26.745	8.437	-0.531	1.00	15.50
8078	CD2	TYR	B	258	-25.410	8.231	-0.184	1.00	14.89
8080	C	TYR	B	258	-23.913	8.839	3.331	1.00	12.18
8081	O	TYR	B	258	-23.773	8.149	4.329	1.00	12.00
8082	N	ASP	B	259	-24.787	9.837	3.239	1.00	11.60
8084	CA	ASP	B	259	-25.586	10.315	4.354	1.00	11.80
8086	CB	ASP	B	259	-24.737	11.192	5.287	1.00	12.13
8089	CG	ASP	B	259	-25.414	11.471	6.626	1.00	12.82
8090	OD1	ASP	B	259	-25.925	12.603	6.835	1.00	13.38
8091	OD2	ASP	B	259	-25.460	10.638	7.545	1.00	15.84
8092	C	ASP	B	259	-26.733	11.155	3.792	1.00	12.11
8093	O	ASP	B	259	-26.710	11.585	2.634	1.00	13.32
8094	N	SER	B	260	-27.716	11.406	4.636	1.00	12.17
8096	CA	SER	B	260	-28.806	12.319	4.307	1.00	12.73
8098	CB	SER	B	260	-29.797	12.378	5.471	1.00	12.53
8101	OG	SER	B	260	-30.616	11.212	5.513	1.00	15.25
8103	C	SER	B	260	-28.305	13.733	4.020	1.00	13.30
8104	O	SER	B	260	-28.916	14.457	3.231	1.00	13.95
8105	N	SER	B	261	-27.210	14.118	4.673	1.00	13.17
8107	CA	SER	B	261	-26.730	15.497	4.676	1.00	13.51
8109	CB	SER	B	261	-26.766	16.051	6.096	1.00	13.96
8112	OG	SER	B	261	-26.317	17.396	6.123	1.00	15.44
8114	C	SER	B	261	-25.307	15.614	4.129	1.00	13.16
8115	O	SER	B	261	-24.430	14.833	4.485	1.00	12.66
8116	N	LEU	B	262	-25.104	16.596	3.259	1.00	13.32
8118	CA	LEU	B	262	-23.778	16.957	2.779	1.00	13.40
8120	CB	LEU	B	262	-23.871	18.007	1.663	1.00	13.97
8123	CG	LEU	B	262	-24.346	17.431	0.326	1.00	16.35
8125	CD1	LEU	B	262	-24.687	18.515	-0.665	1.00	18.16
8129	CD2	LEU	B	262	-23.302	16.480	-0.262	1.00	19.16
8133	C	LEU	B	262	-22.899	17.482	3.908	1.00	12.51
8134	O	LEU	B	262	-21.678	17.421	3.815	1.00	11.68
8135	N	TRP	B	263	-23.505	17.989	4.981	1.00	11.84
8137	CA	TRP	B	263	-22.730	18.386	6.155	1.00	11.33
8139	CB	TRP	B	263	-23.630	18.952	7.262	1.00	11.33
8142	CG	TRP	B	263	-24.111	20.331	6.992	1.00	10.42
8143	CD1	TRP	B	263	-25.155	20.701	6.189	1.00	11.81
8145	NE1	TRP	B	263	-25.285	22.069	6.176	1.00	13.12
8147	CE2	TRP	B	263	-24.326	22.613	6.990	1.00	10.72
8148	CD2	TRP	B	263	-23.564	21.549	7.514	1.00	10.82
8149	CE3	TRP	B	263	-22.509	21.846	8.381	1.00	11.14
8151	CZ3	TRP	B	263	-22.246	23.174	8.681	1.00	11.04
8153	CH2	TRP	B	263	-23.018	24.201	8.139	1.00	11.20
8155	CZ2	TRP	B	263	-24.060	23.940	7.293	1.00	11.38
8157	C	TRP	B	263	-21.949	17.190	6.689	1.00	11.26

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
8158	O	TRP	B	263	-20.805	17.310	7.089	1.00	12.27
8159	N	THR	B	264	-22.577	16.024	6.687	1.00	10.81
8161	CA	THR	B	264	-21.925	14.824	7.159	1.00	11.18
8163	CB	THR	B	264	-22.955	13.727	7.376	1.00	11.47
8165	OG1	THR	B	264	-23.962	14.192	8.279	1.00	12.43
8167	CG2	THR	B	264	-22.295	12.504	8.049	1.00	11.97
8171	C	THR	B	264	-20.884	14.323	6.181	1.00	11.34
8172	O	THR	B	264	-19.744	14.111	6.563	1.00	12.15
8173	N	THR	B	265	-21.272	14.127	4.930	1.00	11.82
8175	CA	THR	B	265	-20.367	13.483	3.983	1.00	12.54
8177	CB	THR	B	265	-21.047	13.141	2.660	1.00	12.86
8179	OG1	THR	B	265	-21.584	14.326	2.063	1.00	13.86
8181	CG2	THR	B	265	-22.235	12.223	2.866	1.00	13.40
8185	C	THR	B	265	-19.145	14.338	3.703	1.00	12.85
8186	O	THR	B	265	-18.068	13.794	3.491	1.00	12.62
8187	N	LEU	B	266	-19.301	15.662	3.686	1.00	12.49
8189	CA	LEU	B	266	-18.165	16.531	3.385	1.00	12.87
8191	CB	LEU	B	266	-18.637	17.874	2.811	1.00	12.67
8194	CG	LEU	B	266	-19.380	17.761	1.470	1.00	14.14
8196	CD1	LEU	B	266	-19.884	19.109	0.995	1.00	14.67
8200	CD2	LEU	B	266	-18.480	17.130	0.405	1.00	16.43
8204	C	LEU	B	266	-17.247	16.734	4.594	1.00	12.76
8205	O	LEU	B	266	-16.029	16.787	4.443	1.00	13.82
8206	N	LEU	B	267	-17.808	16.840	5.793	1.00	12.75
8208	CA	LEU	B	267	-16.995	17.126	6.973	1.00	13.15
8210	CB	LEU	B	267	-17.809	17.871	8.051	1.00	13.10
8213	CG	LEU	B	267	-18.244	19.300	7.685	1.00	14.02
8215	CD1	LEU	B	267	-19.246	19.818	8.700	1.00	14.09
8219	CD2	LEU	B	267	-17.055	20.245	7.583	1.00	15.58
8223	C	LEU	B	267	-16.326	15.901	7.582	1.00	13.40
8224	O	LEU	B	267	-15.281	16.039	8.210	1.00	14.20
8225	N	ILE	B	268	-16.907	14.713	7.399	1.00	14.15
8227	CA	ILE	B	268	-16.326	13.485	7.946	1.00	15.57
8229	CB	ILE	B	268	-17.370	12.323	7.960	1.00	16.26
8231	CG1	ILE	B	268	-16.872	11.152	8.801	1.00	18.86
8234	CD1	ILE	B	268	-17.039	11.367	10.259	1.00	21.64
8238	CG2	ILE	B	268	-17.633	11.828	6.563	1.00	17.50
8242	C	ILE	B	268	-15.085	13.047	7.175	1.00	16.30
8243	O	ILE	B	268	-14.234	12.332	7.706	1.00	15.96
8244	N	ARG	B	269	-14.966	13.456	5.919	1.00	17.45
8246	CA	ARG	B	269	-13.778	13.069	5.176	1.00	18.43
8248	CB	ARG	B	269	-13.946	13.293	3.670	1.00	19.93
8251	CG	ARG	B	269	-13.635	14.661	3.181	1.00	23.73
8254	CD	ARG	B	269	-14.071	14.881	1.733	1.00	28.73
8257	NE	ARG	B	269	-15.463	14.475	1.550	1.00	32.05
8259	CZ	ARG	B	269	-15.929	13.681	0.586	1.00	34.04
8260	NH1	ARG	B	269	-17.223	13.394	0.556	1.00	34.03
8263	NH2	ARG	B	269	-15.128	13.180	-0.355	1.00	35.66
8266	C	ARG	B	269	-12.564	13.784	5.763	1.00	17.41

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
8267	O	ARG	B	269	-12.664	14.883	6.320	1.00	17.41
8268	N	ASN	B	270	-11.425	13.106	5.677	1.00	16.66
8270	CA	ASN	B	270	-10.193	13.521	6.326	1.00	15.94
8272	CB	ASN	B	270	-9.897	12.545	7.489	1.00	15.91
8275	CG	ASN	B	270	-8.634	12.881	8.283	1.00	15.90
8276	OD1	ASN	B	270	-8.224	12.104	9.166	1.00	16.27
8277	ND2	ASN	B	270	-8.028	14.017	8.006	1.00	14.28
8280	C	ASN	B	270	-9.079	13.526	5.286	1.00	15.83
8281	O	ASN	B	270	-8.212	12.640	5.285	1.00	15.02
8282	N	PRO	B	271	-9.088	14.511	4.380	1.00	15.13
8283	CA	PRO	B	271	-8.068	14.560	3.323	1.00	14.80
8285	CB	PRO	B	271	-8.475	15.776	2.490	1.00	15.03
8288	CG	PRO	B	271	-9.275	16.600	3.396	1.00	15.15
8291	CD	PRO	B	271	-10.030	15.637	4.271	1.00	15.28
8294	C	PRO	B	271	-6.655	14.719	3.860	1.00	14.35
8295	O	PRO	B	271	-5.725	14.306	3.177	1.00	14.29
8296	N	SER	B	272	-6.496	15.301	5.044	1.00	13.66
8298	CA	SER	B	272	-5.184	15.443	5.653	1.00	13.66
8300	CB	SER	B	272	-5.269	16.281	6.930	1.00	14.30
8303	OG	SER	B	272	-5.549	17.637	6.602	1.00	17.01
8305	C	SER	B	272	-4.523	14.104	5.931	1.00	13.18
8306	O	SER	B	272	-3.322	13.968	5.782	1.00	13.09
8307	N	ARG	B	273	-5.307	13.103	6.327	1.00	12.74
8309	CA	ARG	B	273	-4.743	11.783	6.544	1.00	12.80
8311	CB	ARG	B	273	-5.798	10.807	7.082	1.00	12.19
8314	CG	ARG	B	273	-5.382	9.356	6.958	1.00	12.13
8317	CD	ARG	B	273	-6.307	8.346	7.673	1.00	11.21
8320	NE	ARG	B	273	-6.277	7.071	6.964	1.00	9.98
8322	CZ	ARG	B	273	-7.137	6.083	7.157	1.00	10.46
8323	NH1	ARG	B	273	-8.058	6.177	8.101	1.00	10.65
8326	NH2	ARG	B	273	-7.061	4.997	6.404	1.00	12.09
8329	C	ARG	B	273	-4.134	11.239	5.259	1.00	13.07
8330	O	ARG	B	273	-3.026	10.717	5.280	1.00	12.90
8331	N	LYS	B	274	-4.867	11.343	4.151	1.00	13.99
8333	CA	LYS	B	274	-4.402	10.802	2.873	1.00	14.94
8335	CB	LYS	B	274	-5.486	10.923	1.794	1.00	16.35
8338	CG	LYS	B	274	-6.712	10.068	2.018	1.00	20.16
8341	CD	LYS	B	274	-7.383	9.742	0.686	1.00	24.62
8344	CE	LYS	B	274	-8.895	9.715	0.789	1.00	26.67
8347	NZ	LYS	B	274	-9.498	9.117	-0.447	1.00	27.18
8351	C	LYS	B	274	-3.142	11.536	2.416	1.00	14.45
8352	O	LYS	B	274	-2.232	10.931	1.863	1.00	13.70
8353	N	ILE	B	275	-3.095	12.841	2.655	1.00	13.49
8355	CA	ILE	B	275	-1.941	13.650	2.282	1.00	13.22
8357	CB	ILE	B	275	-2.264	15.167	2.426	1.00	13.26
8359	CG1	ILE	B	275	-3.091	15.610	1.214	1.00	14.51
8362	CD1	ILE	B	275	-3.862	16.896	1.422	1.00	16.05
8366	CG2	ILE	B	275	-0.981	15.986	2.585	1.00	12.85
8370	C	ILE	B	275	-0.712	13.241	3.096	1.00	13.24

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
8371	O	ILE	B	275	0.355	13.070	2.532	1.00	12.67
8372	N	LEU	B	276	-0.853	13.067	4.407	1.00	13.15
8374	CA	LEU	B	276	0.285	12.656	5.237	1.00	13.49
8376	CB	LEU	B	276	-0.054	12.684	6.724	1.00	14.39
8379	CG	LEU	B	276	-0.126	14.011	7.449	1.00	16.17
8381	CD1	LEU	B	276	-0.511	13.716	8.892	1.00	17.23
8385	CD2	LEU	B	276	1.185	14.776	7.372	1.00	16.43
8389	C	LEU	B	276	0.771	11.250	4.884	1.00	13.17
8390	O	LEU	B	276	1.963	10.991	4.870	1.00	12.63
8391	N	GLU	B	277	-0.153	10.340	4.594	1.00	12.96
8393	CA	GLU	B	277	0.246	9.002	4.169	1.00	12.89
8395	CB	GLU	B	277	-0.978	8.129	3.895	1.00	12.80
8398	CG	GLU	B	277	-1.724	7.735	5.151	1.00	12.57
8401	CD	GLU	B	277	-3.085	7.117	4.888	1.00	13.04
8402	OE1	GLU	B	277	-3.760	6.743	5.863	1.00	12.09
8403	OE2	GLU	B	277	-3.504	7.003	3.716	1.00	14.22
8404	C	GLU	B	277	1.103	9.097	2.920	1.00	13.20
8405	O	GLU	B	277	2.126	8.422	2.806	1.00	13.71
8406	N	PHE	B	278	0.686	9.939	1.981	1.00	13.73
8408	CA	PHE	B	278	1.447	10.105	0.748	1.00	14.82
8410	CB	PHE	B	278	0.710	10.985	-0.259	1.00	14.65
8413	CG	PHE	B	278	1.571	11.385	-1.420	1.00	16.88
8414	CD1	PHE	B	278	1.828	10.487	-2.444	1.00	20.02
8416	CE1	PHE	B	278	2.651	10.850	-3.513	1.00	20.53
8418	CZ	PHE	B	278	3.226	12.106	-3.545	1.00	20.84
8420	CE2	PHE	B	278	2.986	13.010	-2.504	1.00	19.97
8422	CD2	PHE	B	278	2.166	12.634	-1.449	1.00	17.67
8424	C	PHE	B	278	2.820	10.697	1.035	1.00	14.55
8425	O	PHE	B	278	3.836	10.194	0.557	1.00	15.16
8426	N	LEU	B	279	2.864	11.773	1.817	1.00	14.35
8428	CA	LEU	B	279	4.125	12.428	2.117	1.00	14.35
8430	CB	LEU	B	279	3.905	13.707	2.919	1.00	13.89
8433	CG	LEU	B	279	3.207	14.816	2.139	1.00	13.96
8435	CD1	LEU	B	279	2.774	15.941	3.080	1.00	12.96
8439	CD2	LEU	B	279	4.108	15.360	1.029	1.00	12.84
8443	C	LEU	B	279	5.075	11.502	2.860	1.00	15.30
8444	O	LEU	B	279	6.283	11.517	2.605	1.00	15.01
8445	N	TYR	B	280	4.529	10.679	3.751	1.00	16.26
8447	CA	TYR	B	280	5.336	9.750	4.528	1.00	17.66
8449	CB	TYR	B	280	4.521	9.118	5.666	1.00	17.55
8452	CG	TYR	B	280	4.191	10.046	6.827	1.00	15.50
8453	CD1	TYR	B	280	3.484	9.575	7.924	1.00	14.31
8455	CE1	TYR	B	280	3.163	10.399	8.984	1.00	13.88
8457	CZ	TYR	B	280	3.534	11.726	8.963	1.00	14.03
8458	OH	TYR	B	280	3.213	12.546	10.026	1.00	16.74
8460	CE2	TYR	B	280	4.229	12.227	7.880	1.00	13.43
8462	CD2	TYR	B	280	4.556	11.395	6.829	1.00	14.11
8464	C	TYR	B	280	5.936	8.686	3.613	1.00	20.05
8465	O	TYR	B	280	7.074	8.281	3.825	1.00	20.38



# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
8466	N	SER	B	281	5.196	8.294	2.578	1.00	22.76
8468	CA	SER	B	281	5.606	7.222	1.666	1.00	25.12
8470	CB	SER	B	281	4.435	6.780	0.777	1.00	25.24
8473	OG	SER	B	281	4.240	7.651	-0.329	1.00	25.80
8475	C	SER	B	281	6.786	7.627	0.797	1.00	27.46
8476	O	SER	B	281	7.565	6.773	0.382	1.00	28.13
8477	N	THR	B	282	6.919	8.927	0.534	1.00	30.00
8479	CA	THR	B	282	8.041	9.442	-0.255	1.00	31.75
8481	CB	THR	B	282	7.786	10.914	-0.715	1.00	31.78
8483	OG1	THR	B	282	7.706	11.795	0.414	1.00	33.17
8485	CG2	THR	B	282	6.437	11.068	-1.410	1.00	32.34
8489	C	THR	B	282	9.379	9.340	0.490	1.00	32.84
8490	O	THR	B	282	10.434	9.494	-0.121	1.00	33.74
8491	N	SER	B	283	9.333	9.071	1.797	1.00	33.83
8493	CA	SER	B	283	10.531	8.957	2.630	1.00	34.45
8495	CB	SER	B	283	10.234	9.404	4.070	1.00	34.79
8498	OG	SER	B	283	11.039	10.506	4.437	1.00	36.40
8500	C	SER	B	283	11.112	7.556	2.700	1.00	34.09
8501	O	SER	B	283	12.291	7.397	3.006	1.00	35.02
8502	N	TYR	B	284	10.295	6.534	2.457	1.00	33.59
8504	CA	TYR	B	284	10.726	5.156	2.689	1.00	32.95
8506	CB	TYR	B	284	9.797	4.474	3.694	1.00	32.12
8509	CG	TYR	B	284	9.654	5.238	4.993	1.00	28.73
8510	CD1	TYR	B	284	8.521	5.994	5.255	1.00	26.22
8512	CE1	TYR	B	284	8.385	6.700	6.448	1.00	24.33
8514	CZ	TYR	B	284	9.398	6.650	7.388	1.00	23.63
8515	OH	TYR	B	284	9.288	7.335	8.566	1.00	21.11
8517	CE2	TYR	B	284	10.536	5.909	7.150	1.00	24.98
8519	CD2	TYR	B	284	10.658	5.207	5.955	1.00	26.04
8521	C	TYR	B	284	10.793	4.339	1.405	1.00	33.85
8522	O	TYR	B	284	10.024	4.569	0.469	1.00	34.22
8523	N	ASN	B	285	11.716	3.378	1.387	1.00	34.62
8525	CA	ASN	B	285	11.962	2.521	0.233	1.00	35.16
8527	CB	ASN	B	285	13.474	2.393	-0.002	1.00	35.69
8530	CG	ASN	B	285	13.821	1.773	-1.353	1.00	36.74
8531	OD1	ASN	B	285	12.946	1.372	-2.118	1.00	38.95
8532	ND2	ASN	B	285	15.117	1.697	-1.648	1.00	39.65
8535	C	ASN	B	285	11.343	1.144	0.459	1.00	35.32
8536	O	ASN	B	285	11.760	0.410	1.359	1.00	35.16
8537	N	MET	B	286	10.355	0.799	-0.366	1.00	35.43
8539	CA	MET	B	286	9.591	-0.438	-0.207	1.00	35.68
8541	CB	MET	B	286	8.128	-0.219	-0.626	1.00	35.78
8544	CG	MET	B	286	7.395	0.860	0.153	1.00	36.06
8547	SD	MET	B	286	7.077	0.401	1.873	1.00	38.05
8548	CE	MET	B	286	8.096	1.588	2.710	1.00	38.26
8552	C	MET	B	286	10.153	-1.622	-1.002	1.00	35.73
8553	O	MET	B	286	9.575	-2.705	-0.958	1.00	35.88
8554	N	ASP	B	287	11.260	-1.424	-1.723	1.00	36.01
8556	CA	ASP	B	287	11.855	-2.484	-2.556	1.00	36.13

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
8558	CB	ASP	B	287	13.152	-1.991	-3.222	1.00	36.54
8561	CG	ASP	B	287	12.899	-1.090	-4.422	1.00	38.05
8562	OD1	ASP	B	287	11.727	-0.934	-4.836	1.00	39.91
8563	OD2	ASP	B	287	13.824	-0.494	-5.021	1.00	40.92
8564	C	ASP	B	287	12.149	-3.745	-1.748	1.00	35.73
8565	O	ASP	B	287	11.867	-4.856	-2.188	1.00	35.62
8566	N	ARG	B	288	12.726	-3.538	-0.567	1.00	35.51
8568	CA	ARG	B	288	12.943	-4.559	0.466	1.00	35.62
8570	CB	ARG	B	288	13.124	-3.814	1.808	1.00	36.14
8573	CG	ARG	B	288	13.509	-4.633	3.022	1.00	37.85
8576	CD	ARG	B	288	13.464	-3.837	4.336	1.00	39.97
8579	NE	ARG	B	288	13.307	-4.721	5.495	1.00	41.73
8581	CZ	ARG	B	288	12.940	-4.335	6.715	1.00	43.08
8582	NH1	ARG	B	288	12.668	-3.058	6.982	1.00	41.03
8585	NH2	ARG	B	288	12.840	-5.250	7.680	1.00	44.66
8588	C	ARG	B	288	11.800	-5.585	0.589	1.00	34.78
8589	O	ARG	B	288	12.039	-6.786	0.741	1.00	34.29
8590	N	PHE	B	289	10.561	-5.100	0.529	1.00	33.96
8592	CA	PHE	B	289	9.376	-5.929	0.784	1.00	33.49
8594	CB	PHE	B	289	8.284	-5.078	1.437	1.00	33.18
8597	CG	PHE	B	289	8.754	-4.338	2.651	1.00	32.18
8598	CD1	PHE	B	289	8.938	-2.964	2.615	1.00	31.36
8600	CE1	PHE	B	289	9.385	-2.276	3.737	1.00	31.08
8602	CZ	PHE	B	289	9.659	-2.966	4.908	1.00	30.78
8604	CE2	PHE	B	289	9.484	-4.340	4.952	1.00	31.52
8606	CD2	PHE	B	289	9.034	-5.021	3.824	1.00	31.95
8608	C	PHE	B	289	8.815	-6.593	-0.463	1.00	33.46
8609	O	PHE	B	289	8.064	-7.567	-0.350	1.00	33.70
8610	N	GLN	C	20	-58.294	-40.530	-19.881	1.00	34.74
8612	CA	GLN	C	20	-58.716	-40.474	-21.311	1.00	33.92
8614	CB	GLN	C	20	-58.639	-39.069	-21.940	1.00	33.64
8617	CG	GLN	C	20	-57.233	-38.613	-22.240	1.00	30.56
8620	CD	GLN	C	20	-56.449	-38.272	-20.994	1.00	26.16
8621	OE1	GLN	C	20	-56.998	-37.722	-20.037	1.00	19.55
8622	NE2	GLN	C	20	-55.161	-38.569	-21.015	1.00	23.79
8625	C	GLN	C	20	-58.703	-41.693	-22.286	1.00	34.23
8626	O	GLN	C	20	-58.210	-42.768	-21.949	1.00	35.14
8630	N	GLN	C	21	-59.251	-41.476	-23.479	1.00	34.08
8632	CA	GLN	C	21	-58.974	-42.319	-24.633	1.00	34.04
8634	CB	GLN	C	21	-60.177	-42.369	-25.578	1.00	34.40
8637	CG	GLN	C	21	-61.117	-43.536	-25.320	1.00	35.52
8640	CD	GLN	C	21	-62.431	-43.395	-26.062	1.00	37.46
8641	OE1	GLN	C	21	-62.518	-43.721	-27.248	1.00	38.85
8642	NE2	GLN	C	21	-63.457	-42.904	-25.370	1.00	38.76
8645	C	GLN	C	21	-57.769	-41.711	-25.354	1.00	33.63
8646	O	GLN	C	21	-57.858	-40.597	-25.884	1.00	33.46
8647	N	PRO	C	22	-56.643	-42.422	-25.369	1.00	32.92
8648	CA	PRO	C	22	-55.456	-41.927	-26.068	1.00	32.63
8650	CB	PRO	C	22	-54.325	-42.796	-25.510	1.00	32.47

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
8653	CG	PRO	C	22	-54.981	-44.065	-25.062	1.00	32.96
8656	CD	PRO	C	22	-56.414	-43.745	-24.763	1.00	32.97
8659	C	PRO	C	22	-55.623	-42.118	-27.572	1.00	32.44
8660	O	PRO	C	22	-56.507	-42.869	-27.998	1.00	32.00
8661	N	LEU	C	23	-54.809	-41.425	-28.360	1.00	32.07
8663	CA	LEU	C	23	-54.842	-41.563	-29.810	1.00	32.03
8665	CB	LEU	C	23	-54.134	-40.381	-30.482	1.00	31.96
8668	CG	LEU	C	23	-54.591	-38.974	-30.085	1.00	32.00
8670	CD1	LEU	C	23	-53.811	-37.925	-30.871	1.00	32.25
8674	CD2	LEU	C	23	-56.094	-38.805	-30.294	1.00	32.10
8678	C	LEU	C	23	-54.153	-42.866	-30.189	1.00	32.18
8679	O	LEU	C	23	-53.012	-43.096	-29.785	1.00	32.36
8680	N	ASN	C	24	-54.855	-43.722	-30.935	1.00	32.33
8682	CA	ASN	C	24	-54.269	-44.956	-31.465	1.00	32.45
8684	CB	ASN	C	24	-55.354	-46.008	-31.764	1.00	32.89
8687	CG	ASN	C	24	-55.890	-46.687	-30.499	1.00	34.04
8688	OD1	ASN	C	24	-55.579	-46.285	-29.375	1.00	36.84
8689	ND2	ASN	C	24	-56.705	-47.723	-30.685	1.00	35.96
8692	C	ASN	C	24	-53.460	-44.617	-32.722	1.00	31.90
8693	O	ASN	C	24	-53.883	-44.884	-33.854	1.00	31.87
8694	N	GLU	C	25	-52.295	-44.008	-32.496	1.00	31.12
8696	CA	GLU	C	25	-51.475	-43.413	-33.555	1.00	30.47
8698	CB	GLU	C	25	-51.908	-41.963	-33.808	1.00	30.75
8701	CG	GLU	C	25	-53.368	-41.775	-34.195	1.00	32.21
8704	CD	GLU	C	25	-53.754	-40.319	-34.374	1.00	33.97
8705	OE1	GLU	C	25	-54.904	-39.968	-34.033	1.00	35.70
8706	OE2	GLU	C	25	-52.921	-39.525	-34.860	1.00	35.50
8707	C	GLU	C	25	-49.992	-43.403	-33.174	1.00	29.30
8708	O	GLU	C	25	-49.638	-43.395	-31.993	1.00	29.30
8709	N	GLU	C	26	-49.129	-43.396	-34.186	1.00	27.68
8711	CA	GLU	C	26	-47.704	-43.169	-33.985	1.00	26.35
8713	CB	GLU	C	26	-46.908	-43.657	-35.203	1.00	26.79
8716	CG	GLU	C	26	-45.414	-43.844	-34.954	1.00	29.24
8719	CD	GLU	C	26	-44.667	-44.403	-36.161	1.00	32.01
8720	OE1	GLU	C	26	-43.503	-43.995	-36.386	1.00	34.80
8721	OE2	GLU	C	26	-45.231	-45.251	-36.889	1.00	34.16
8722	C	GLU	C	26	-47.515	-41.667	-33.798	1.00	24.05
8723	O	GLU	C	26	-48.145	-40.876	-34.501	1.00	23.56
8724	N	PHE	C	27	-46.672	-41.270	-32.847	1.00	21.62
8726	CA	PHE	C	27	-46.326	-39.860	-32.700	1.00	19.65
8728	CB	PHE	C	27	-45.439	-39.592	-31.475	1.00	19.28
8731	CG	PHE	C	27	-44.962	-38.164	-31.393	1.00	16.57
8732	CD1	PHE	C	27	-43.707	-37.798	-31.863	1.00	15.23
8734	CE1	PHE	C	27	-43.292	-36.476	-31.823	1.00	14.65
8736	CZ	PHE	C	27	-44.134	-35.498	-31.316	1.00	14.61
8738	CE2	PHE	C	27	-45.384	-35.848	-30.861	1.00	14.24
8740	CD2	PHE	C	27	-45.799	-37.171	-30.903	1.00	14.62
8742	C	PHE	C	27	-45.582	-39.391	-33.940	1.00	18.77
8743	O	PHE	C	27	-44.716	-40.095	-34.455	1.00	18.59

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
8744	N	ARG	C	28	-45.919	-38.198	-34.418	1.00	17.61
8746	CA	ARG	C	28	-45.074	-37.503	-35.379	1.00	17.40
8748	CB	ARG	C	28	-45.621	-37.622	-36.805	1.00	18.04
8751	CG	BARG	C	28	-46.908	-36.841	-37.052	0.35	19.02
8752	CG	AARG	C	28	-46.898	-36.858	-37.058	0.65	20.07
8757	CD	BARG	C	28	-47.652	-37.222	-38.327	0.35	20.33
8758	CD	AARG	C	28	-47.769	-37.475	-38.132	0.65	22.53
8763	NE	BARG	C	28	-49.069	-37.494	-38.069	0.35	20.89
8764	NE	AARG	C	28	-48.263	-38.791	-37.722	0.65	23.73
8767	CZ	BARG	C	28	-50.050	-36.595	-38.124	0.35	21.86
8768	CZ	AARG	C	28	-49.494	-39.052	-37.290	0.65	24.81
8769	NH1	BARG	C	28	-51.296	-36.974	-37.871	0.35	22.22
8770	NH1	AARG	C	28	-50.417	-38.094	-37.201	0.65	25.76
8775	NH2	BARG	C	28	-49.808	-35.323	-38.424	0.35	22.88
8776	NH2	AARG	C	28	-49.811	-40.297	-36.951	0.65	25.62
8781	C	ARG	C	28	-44.968	-36.046	-34.960	1.00	16.08
8782	O	ARG	C	28	-45.919	-35.509	-34.387	1.00	14.94
8783	N	PRO	C	29	-43.824	-35.411	-35.219	1.00	15.89
8784	CA	PRO	C	29	-43.629	-34.021	-34.791	1.00	15.52
8786	CB	PRO	C	29	-42.209	-33.697	-35.250	1.00	15.90
8789	CG	PRO	C	29	-41.884	-34.705	-36.265	1.00	16.44
8792	CD	PRO	C	29	-42.629	-35.944	-35.892	1.00	15.85
8795	C	PRO	C	29	-44.622	-33.044	-35.396	1.00	15.17
8796	O	PRO	C	29	-44.833	-31.989	-34.818	1.00	14.21
8797	N	GLU	C	30	-45.220	-33.388	-36.534	1.00	14.88
8799	CA	GLU	C	30	-46.200	-32.516	-37.180	1.00	14.90
8801	CB	GLU	C	30	-46.507	-33.005	-38.606	1.00	15.12
8804	CG	GLU	C	30	-45.343	-32.842	-39.573	1.00	16.80
8807	CD	GLU	C	30	-44.191	-33.810	-39.349	1.00	17.15
8808	OE1	GLU	C	30	-43.039	-33.422	-39.635	1.00	18.60
8809	OE2	GLU	C	30	-44.413	-34.954	-38.883	1.00	19.19
8810	C	GLU	C	30	-47.488	-32.384	-36.372	1.00	14.30
8811	O	GLU	C	30	-48.276	-31.480	-36.610	1.00	14.68
8812	N	MET	C	31	-47.691	-33.272	-35.401	1.00	13.87
8814	CA	MET	C	31	-48.788	-33.137	-34.445	1.00	13.81
8816	CB	MET	C	31	-48.771	-34.310	-33.460	1.00	13.99
8819	CG	MET	C	31	-49.217	-35.622	-34.067	1.00	14.31
8822	SD	MET	C	31	-49.025	-36.994	-32.932	1.00	16.13
8823	CE	MET	C	31	-50.136	-38.189	-33.639	1.00	16.41
8827	C	MET	C	31	-48.760	-31.817	-33.663	1.00	13.62
8828	O	MET	C	31	-49.797	-31.361	-33.157	1.00	14.44
8829	N	LEU	C	32	-47.582	-31.212	-33.542	1.00	12.84
8831	CA	LEU	C	32	-47.429	-29.967	-32.793	1.00	12.41
8833	CB	LEU	C	32	-46.208	-30.045	-31.867	1.00	12.16
8836	CG	LEU	C	32	-46.390	-30.739	-30.510	1.00	13.21
8838	CD1	LEU	C	32	-46.715	-32.207	-30.703	1.00	14.47
8842	CD2	LEU	C	32	-47.451	-30.037	-29.675	1.00	13.75
8846	C	LEU	C	32	-47.311	-28.749	-33.705	1.00	12.13
8847	O	LEU	C	32	-47.226	-27.628	-33.238	1.00	12.23

## FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
8848	N	GLN	C	33	-47.292	-28.977	-35.010	1.00	11.56
8850	CA	GLN	C	33	-47.152	-27.888	-35.972	1.00	12.02
8852	CB	GLN	C	33	-47.065	-28.474	-37.374	1.00	12.50
8855	CG	GLN	C	33	-46.679	-27.489	-38.445	1.00	13.47
8858	CD	GLN	C	33	-46.534	-28.171	-39.802	1.00	15.42
8859	OE1	GLN	C	33	-45.630	-28.979	-39.994	1.00	17.41
8860	NE2	GLN	C	33	-47.428	-27.856	-40.729	1.00	15.74
8863	C	GLN	C	33	-48.319	-26.908	-35.888	1.00	11.74
8864	O	GLN	C	33	-49.475	-27.297	-36.047	1.00	12.39
8865	N	GLY	C	34	-48.014	-25.643	-35.605	1.00	11.29
8867	CA	GLY	C	34	-49.024	-24.608	-35.459	1.00	11.07
8870	C	GLY	C	34	-49.833	-24.662	-34.173	1.00	10.89
8871	O	GLY	C	34	-50.736	-23.847	-33.969	1.00	11.58
8872	N	LYS	C	35	-49.515	-25.605	-33.297	1.00	11.09
8874	CA	LYS	C	35	-50.224	-25.719	-32.033	1.00	11.12
8876	CB	LYS	C	35	-50.042	-27.105	-31.416	1.00	11.33
8879	CG	LYS	C	35	-50.649	-28.260	-32.222	1.00	13.18
8882	CD	LYS	C	35	-52.160	-28.163	-32.298	1.00	15.59
8885	CE	LYS	C	35	-52.774	-29.389	-32.993	1.00	18.26
8888	NZ	LYS	C	35	-54.264	-29.302	-33.053	1.00	22.35
8892	C	LYS	C	35	-49.718	-24.645	-31.094	1.00	10.85
8893	O	LYS	C	35	-48.576	-24.212	-31.185	1.00	11.64
8894	N	LYS	C	36	-50.579	-24.222	-30.180	1.00	10.28
8896	CA	LYS	C	36	-50.316	-23.095	-29.288	1.00	10.30
8898	CB	LYS	C	36	-51.523	-22.148	-29.324	1.00	10.46
8901	CG	LYS	C	36	-51.745	-21.593	-30.724	1.00	11.20
8904	CD	LYS	C	36	-53.107	-21.004	-30.941	1.00	13.10
8907	CE	LYS	C	36	-53.188	-20.561	-32.409	1.00	15.63
8910	NZ	LYS	C	36	-54.478	-19.927	-32.742	1.00	18.66
8914	C	LYS	C	36	-50.057	-23.664	-27.898	1.00	10.34
8915	O	LYS	C	36	-50.935	-24.236	-27.281	1.00	10.38
8916	N	VAL	C	37	-48.820	-23.538	-27.438	1.00	9.90
8918	CA	VAL	C	37	-48.351	-24.266	-26.262	1.00	9.42
8920	CB	VAL	C	37	-47.325	-25.366	-26.648	1.00	9.26
8922	CG1	VAL	C	37	-46.985	-26.231	-25.432	1.00	9.38
8926	CG2	VAL	C	37	-47.849	-26.206	-27.795	1.00	10.02
8930	C	VAL	C	37	-47.701	-23.342	-25.231	1.00	9.79
8931	O	VAL	C	37	-46.835	-22.529	-25.563	1.00	10.00
8932	N	ILE	C	38	-48.154	-23.449	-23.988	1.00	9.17
8934	CA	ILE	C	38	-47.484	-22.853	-22.839	1.00	9.27
8936	CB	ILE	C	38	-48.513	-22.426	-21.769	1.00	9.39
8938	CG1	ILE	C	38	-49.227	-21.147	-22.203	1.00	9.78
8941	CD1	ILE	C	38	-50.414	-20.801	-21.363	1.00	11.02
8945	CG2	ILE	C	38	-47.882	-22.292	-20.357	1.00	9.47
8949	C	ILE	C	38	-46.525	-23.869	-22.256	1.00	9.61
8950	O	ILE	C	38	-46.899	-25.022	-22.052	1.00	9.66
8951	N	VAL	C	39	-45.294	-23.445	-21.978	1.00	9.16
8953	CA	VAL	C	39	-44.377	-24.251	-21.176	1.00	9.38
8955	CB	VAL	C	39	-43.123	-24.705	-21.946	1.00	9.89

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
8957	CG1	VAL	C	39	-42.354	-25.735	-21.137	1.00	10.83
8961	CG2	VAL	C	39	-43.488	-25.241	-23.312	1.00	11.16
8965	C	VAL	C	39	-43.941	-23.450	-19.954	1.00	9.46
8966	O	VAL	C	39	-43.358	-22.379	-20.094	1.00	9.23
8967	N	THR	C	40	-44.224	-23.956	-18.758	1.00	8.93
8969	CA	THR	C	40	-43.726	-23.314	-17.534	1.00	9.10
8971	CB	THR	C	40	-44.756	-23.322	-16.376	1.00	9.12
8973	OG1	THR	C	40	-44.857	-24.633	-15.785	1.00	10.21
8975	CG2	THR	C	40	-46.151	-22.930	-16.852	1.00	9.30
8979	C	THR	C	40	-42.409	-23.939	-17.082	1.00	8.88
8980	O	THR	C	40	-42.033	-25.023	-17.543	1.00	9.42
8981	N	GLY	C	41	-41.674	-23.220	-16.243	1.00	8.58
8983	CA	GLY	C	41	-40.349	-23.649	-15.835	1.00	8.78
8986	C	GLY	C	41	-39.460	-23.901	-17.038	1.00	9.70
8987	O	GLY	C	41	-38.798	-24.933	-17.124	1.00	9.56
8988	N	ALA	C	42	-39.419	-22.935	-17.949	1.00	9.58
8990	CA	ALA	C	42	-38.818	-23.146	-19.269	1.00	10.14
8992	CB	ALA	C	42	-39.841	-22.817	-20.353	1.00	10.78
8996	C	ALA	C	42	-37.525	-22.374	-19.491	1.00	10.71
8997	O	ALA	C	42	-36.999	-22.341	-20.622	1.00	11.74
8998	N	SER	C	43	-36.974	-21.787	-18.435	1.00	11.03
9000	CA	SER	C	43	-35.695	-21.080	-18.549	1.00	11.33
9002	CB	SER	C	43	-35.524	-20.045	-17.435	1.00	11.39
9005	OG	SER	C	43	-35.562	-20.642	-16.158	1.00	11.36
9007	C	SER	C	43	-34.499	-22.035	-18.544	1.00	12.10
9008	O	SER	C	43	-33.426	-21.692	-19.028	1.00	12.13
9009	N	LYS	C	44	-34.674	-23.220	-17.980	1.00	11.92
9011	CA	LYS	C	44	-33.599	-24.215	-17.933	1.00	12.09
9013	CB	LYS	C	44	-32.651	-23.905	-16.781	1.00	13.06
9016	CG	LYS	C	44	-33.288	-23.932	-15.419	1.00	13.91
9019	CD	LYS	C	44	-32.326	-23.440	-14.337	1.00	16.38
9022	CE	LYS	C	44	-32.944	-23.533	-12.945	1.00	17.60
9025	NZ	LYS	C	44	-31.966	-23.049	-11.895	1.00	18.30
9029	C	LYS	C	44	-34.180	-25.610	-17.788	1.00	11.80
9030	O	LYS	C	44	-35.390	-25.787	-17.799	1.00	11.61
9031	N	GLY	C	45	-33.307	-26.600	-17.678	1.00	11.96
9033	CA	GLY	C	45	-33.736	-27.960	-17.417	1.00	11.30
9036	C	GLY	C	45	-34.611	-28.561	-18.496	1.00	11.07
9037	O	GLY	C	45	-34.506	-28.221	-19.685	1.00	10.93
9038	N	ILE	C	46	-35.514	-29.434	-18.066	1.00	10.70
9040	CA	ILE	C	46	-36.425	-30.131	-18.964	1.00	10.28
9042	CB	ILE	C	46	-37.210	-31.205	-18.181	1.00	10.39
9044	CG1	ILE	C	46	-36.266	-32.274	-17.605	1.00	11.07
9047	CD1	ILE	C	46	-36.799	-32.947	-16.344	1.00	12.06
9051	CG2	ILE	C	46	-38.248	-31.872	-19.070	1.00	12.00
9055	C	ILE	C	46	-37.370	-29.154	-19.696	1.00	10.06
9056	O	ILE	C	46	-37.671	-29.328	-20.869	1.00	10.64
9057	N	GLY	C	47	-37.826	-28.121	-19.003	1.00	9.73
9059	CA	GLY	C	47	-38.747	-27.166	-19.597	1.00	9.86

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
9062	C	GLY	C	47	-38.144	-26.442	-20.779	1.00	9.83
9063	O	GLY	C	47	-38.806	-26.245	-21.784	1.00	9.75
9064	N	ARG	C	48	-36.892	-26.020	-20.636	1.00	9.89
9066	CA	ARG	C	48	-36.186	-25.372	-21.735	1.00	10.00
9068	CB	ARG	C	48	-34.784	-24.919	-21.307	1.00	10.57
9071	CG	ARG	C	48	-33.968	-24.327	-22.462	1.00	12.41
9074	CD	ARG	C	48	-32.694	-23.612	-22.012	1.00	15.48
9077	NE	ARG	C	48	-31.799	-24.489	-21.279	1.00	19.90
9079	CZ	ARG	C	48	-30.885	-24.081	-20.390	1.00	21.69
9080	NH1	ARG	C	48	-30.726	-22.785	-20.081	1.00	22.79
9083	NH2	ARG	C	48	-30.134	-24.983	-19.782	1.00	22.98
9086	C	ARG	C	48	-36.088	-26.333	-22.913	1.00	10.04
9087	O	ARG	C	48	-36.324	-25.955	-24.055	1.00	9.50
9088	N	GLU	C	49	-35.749	-27.586	-22.640	1.00	9.52
9090	CA	GLU	C	49	-35.648	-28.567	-23.712	1.00	10.42
9092	CB	GLU	C	49	-35.050	-29.880	-23.202	1.00	10.62
9095	CG	GLU	C	49	-33.621	-29.754	-22.658	1.00	13.07
9098	CD	GLU	C	49	-32.648	-29.075	-23.622	1.00	16.89
9099	OE1	GLU	C	49	-31.837	-28.222	-23.173	1.00	19.30
9100	OE2	GLU	C	49	-32.681	-29.384	-24.842	1.00	19.75
9101	C	GLU	C	49	-36.988	-28.801	-24.398	1.00	10.05
9102	O	GLU	C	49	-37.044	-29.018	-25.601	1.00	10.17
9103	N	MET	C	50	-38.078	-28.750	-23.644	1.00	9.36
9105	CA	MET	C	50	-39.406	-28.896	-24.243	1.00	9.62
9107	CB	MET	C	50	-40.492	-29.042	-23.162	1.00	9.98
9110	CG	MET	C	50	-40.469	-30.405	-22.496	1.00	10.30
9113	SD	MET	C	50	-41.882	-30.737	-21.419	1.00	11.40
9114	CE	MET	C	50	-41.552	-29.666	-20.060	1.00	11.95
9118	C	MET	C	50	-39.717	-27.721	-25.172	1.00	9.95
9119	O	MET	C	50	-40.227	-27.918	-26.264	1.00	10.16
9120	N	ALA	C	51	-39.396	-26.506	-24.733	1.00	10.28
9122	CA	ALA	C	51	-39.552	-25.318	-25.576	1.00	10.22
9124	CB	ALA	C	51	-39.086	-24.072	-24.852	1.00	10.32
9128	C	ALA	C	51	-38.810	-25.484	-26.898	1.00	10.37
9129	O	ALA	C	51	-39.368	-25.214	-27.953	1.00	10.15
9130	N	TYR	C	52	-37.566	-25.947	-26.842	1.00	10.10
9132	CA	TYR	C	52	-36.773	-26.146	-28.052	1.00	10.14
9134	CB	TYR	C	52	-35.322	-26.452	-27.682	1.00	10.18
9137	CG	TYR	C	52	-34.545	-25.310	-27.060	1.00	10.31
9138	CD1	TYR	C	52	-35.020	-24.000	-27.072	1.00	10.91
9140	CE1	TYR	C	52	-34.289	-22.964	-26.514	1.00	12.38
9142	CZ	TYR	C	52	-33.090	-23.223	-25.920	1.00	13.51
9143	OH	TYR	C	52	-32.376	-22.170	-25.370	1.00	17.22
9145	CE2	TYR	C	52	-32.592	-24.502	-25.881	1.00	12.99
9147	CD2	TYR	C	52	-33.319	-25.545	-26.448	1.00	12.38
9149	C	TYR	C	52	-37.347	-27.214	-28.983	1.00	10.50
9150	O	TYR	C	52	-37.388	-27.012	-30.198	1.00	10.63
9151	N	HIS	C	53	-37.804	-28.338	-28.439	1.00	10.28
9153	CA	HIS	C	53	-38.446	-29.365	-29.259	1.00	10.56

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
9155	CB	HIS	C	53	-38.830	-30.595	-28.450	1.00	11.10
9158	CG	HIS	C	53	-37.703	-31.537	-28.189	1.00	11.49
9159	ND1	HIS	C	53	-36.989	-32.148	-29.201	1.00	13.66
9161	CE1	HIS	C	53	-36.082	-32.946	-28.665	1.00	13.86
9163	NE2	HIS	C	53	-36.190	-32.882	-27.351	1.00	14.64
9165	CD2	HIS	C	53	-37.203	-32.017	-27.027	1.00	13.26
9167	C	HIS	C	53	-39.697	-28.812	-29.936	1.00	10.34
9168	O	HIS	C	53	-39.898	-29.031	-31.125	1.00	10.57
9169	N	LEU	C	54	-40.528	-28.098	-29.184	1.00	9.83
9171	CA	LEU	C	54	-41.743	-27.505	-29.722	1.00	9.97
9173	CB	LEU	C	54	-42.542	-26.819	-28.609	1.00	10.09
9176	CG	LEU	C	54	-43.180	-27.801	-27.624	1.00	10.41
9178	CD1	LEU	C	54	-43.573	-27.108	-26.349	1.00	10.61
9182	CD2	LEU	C	54	-44.366	-28.525	-28.244	1.00	11.32
9186	C	LEU	C	54	-41.425	-26.515	-30.840	1.00	10.00
9187	O	LEU	C	54	-42.104	-26.469	-31.869	1.00	10.01
9188	N	ALA	C	55	-40.372	-25.740	-30.640	1.00	10.04
9190	CA	ALA	C	55	-39.931	-24.776	-31.634	1.00	9.96
9192	CB	ALA	C	55	-38.780	-23.945	-31.085	1.00	10.11
9196	C	ALA	C	55	-39.525	-25.482	-32.930	1.00	10.21
9197	O	ALA	C	55	-39.957	-25.096	-34.010	1.00	10.50
9198	N	LYS	C	56	-38.746	-26.552	-32.815	1.00	10.86
9200	CA	LYS	C	56	-38.371	-27.358	-33.974	1.00	12.10
9202	CB	LYS	C	56	-37.400	-28.466	-33.571	1.00	13.15
9205	CG	LYS	C	56	-36.026	-27.987	-33.176	1.00	17.15
9208	CD	LYS	C	56	-35.086	-29.152	-32.868	1.00	21.41
9211	CE	LYS	C	56	-34.119	-28.830	-31.731	1.00	24.71
9214	NZ	LYS	C	56	-34.636	-29.204	-30.384	1.00	27.93
9218	C	LYS	C	56	-39.578	-27.952	-34.707	1.00	11.97
9219	O	LYS	C	56	-39.547	-28.104	-35.941	1.00	12.71
9220	N	MET	C	57	-40.639	-28.277	-33.966	1.00	11.66
9222	CA	MET	C	57	-41.874	-28.797	-34.545	1.00	11.34
9224	CB	MET	C	57	-42.659	-29.592	-33.497	1.00	11.80
9227	CG	MET	C	57	-41.920	-30.812	-32.956	1.00	12.52
9230	SD	MET	C	57	-42.761	-31.490	-31.494	1.00	16.13
9231	CE	MET	C	57	-41.557	-32.632	-30.857	1.00	16.25
9235	C	MET	C	57	-42.777	-27.721	-35.163	1.00	10.82
9236	O	MET	C	57	-43.803	-28.043	-35.754	1.00	11.20
9237	N	GLY	C	58	-42.419	-26.453	-35.015	1.00	10.40
9239	CA	GLY	C	58	-43.187	-25.375	-35.601	1.00	10.33
9242	C	GLY	C	58	-44.387	-24.942	-34.779	1.00	10.39
9243	O	GLY	C	58	-45.353	-24.418	-35.329	1.00	10.94
9244	N	ALA	C	59	-44.338	-25.188	-33.477	1.00	10.05
9246	CA	ALA	C	59	-45.376	-24.706	-32.575	1.00	10.08
9248	CB	ALA	C	59	-45.350	-25.477	-31.268	1.00	10.26
9252	C	ALA	C	59	-45.237	-23.216	-32.308	1.00	9.86
9253	O	ALA	C	59	-44.166	-22.628	-32.497	1.00	9.56
9254	N	HIS	C	60	-46.345	-22.616	-31.869	1.00	9.96
9256	CA	HIS	C	60	-46.341	-21.334	-31.170	1.00	10.37



# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
9258	CB	HIS	C	60	-47.703	-20.657	-31.253	1.00	10.97
9261	CG	HIS	C	60	-48.114	-20.262	-32.637	1.00	11.54
9262	ND1	HIS	C	60	-47.765	-19.051	-33.194	1.00	10.89
9264	CE1	HIS	C	60	-48.290	-18.961	-34.405	1.00	11.52
9266	NE2	HIS	C	60	-48.976	-20.065	-34.649	1.00	11.71
9268	CD2	HIS	C	60	-48.896	-20.887	-33.550	1.00	11.20
9270	C	HIS	C	60	-46.059	-21.635	-29.714	1.00	10.75
9271	O	HIS	C	60	-46.682	-22.521	-29.155	1.00	10.58
9272	N	VAL	C	61	-45.124	-20.912	-29.103	1.00	10.62
9274	CA	VAL	C	61	-44.782	-21.152	-27.698	1.00	11.59
9276	CB	VAL	C	61	-43.422	-21.872	-27.536	1.00	12.02
9278	CG1	VAL	C	61	-43.413	-23.172	-28.306	1.00	13.77
9282	CG2	VAL	C	61	-42.272	-20.992	-27.965	1.00	13.73
9286	C	VAL	C	61	-44.770	-19.885	-26.876	1.00	11.39
9287	O	VAL	C	61	-44.349	-18.826	-27.350	1.00	11.45
9288	N	VAL	C	62	-45.284	-19.981	-25.649	1.00	10.43
9290	CA	VAL	C	62	-45.062	-18.966	-24.637	1.00	10.88
9292	CB	VAL	C	62	-46.368	-18.272	-24.196	1.00	10.32
9294	CG1	VAL	C	62	-46.098	-17.223	-23.120	1.00	11.49
9298	CG2	VAL	C	62	-47.036	-17.621	-25.388	1.00	11.11
9302	C	VAL	C	62	-44.403	-19.667	-23.466	1.00	10.82
9303	O	VAL	C	62	-44.950	-20.628	-22.933	1.00	11.68
9304	N	VAL	C	63	-43.232	-19.172	-23.088	1.00	10.56
9306	CA	VAL	C	63	-42.441	-19.746	-22.010	1.00	10.42
9308	CB	VAL	C	63	-40.979	-20.024	-22.441	1.00	10.74
9310	CG1	VAL	C	63	-40.297	-18.787	-23.008	1.00	10.69
9314	CG2	VAL	C	63	-40.962	-21.154	-23.448	1.00	11.36
9318	C	VAL	C	63	-42.483	-18.822	-20.796	1.00	10.47
9319	O	VAL	C	63	-42.628	-17.607	-20.922	1.00	10.36
9320	N	THR	C	64	-42.387	-19.408	-19.609	1.00	9.23
9322	CA	THR	C	64	-42.310	-18.624	-18.392	1.00	9.70
9324	CB	THR	C	64	-43.726	-18.332	-17.835	1.00	9.90
9326	OG1	THR	C	64	-43.650	-17.466	-16.701	1.00	10.69
9328	CG2	THR	C	64	-44.431	-19.590	-17.362	1.00	10.15
9332	C	THR	C	64	-41.394	-19.291	-17.381	1.00	9.61
9333	O	THR	C	64	-41.122	-20.492	-17.464	1.00	10.11
9334	N	ALA	C	65	-40.888	-18.447	-16.488	1.00	9.43
9336	CA	ALA	C	65	-40.030	-18.763	-15.341	1.00	9.33
9338	CB	ALA	C	65	-38.748	-19.466	-15.790	1.00	9.95
9342	C	ALA	C	65	-39.741	-17.386	-14.705	1.00	9.61
9343	O	ALA	C	65	-40.263	-16.375	-15.175	1.00	9.33
9344	N	ARG	C	66	-38.920	-17.327	-13.662	1.00	9.34
9346	CA	ARG	C	66	-38.539	-16.032	-13.093	1.00	9.67
9348	CB	ARG	C	66	-38.040	-16.192	-11.667	1.00	9.72
9351	CG	ARG	C	66	-39.074	-16.779	-10.709	1.00	10.29
9354	CD	ARG	C	66	-38.483	-17.237	-9.401	1.00	11.04
9357	NE	ARG	C	66	-37.459	-18.247	-9.633	1.00	12.29
9359	CZ	ARG	C	66	-36.557	-18.633	-8.743	1.00	13.19
9360	NH1	ARG	C	66	-35.660	-19.538	-9.075	1.00	13.27

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
9363	NH2	ARG	C	66	-36.544	-18.124	-7.518	1.00	15.60
9366	C	ARG	C	66	-37.468	-15.298	-13.909	1.00	10.07
9367	O	ARG	C	66	-37.443	-14.075	-13.892	1.00	10.35
9368	N	SER	C	67	-36.610	-16.044	-14.607	1.00	9.93
9370	CA	SER	C	67	-35.374	-15.502	-15.179	1.00	10.92
9372	CB	SER	C	67	-34.346	-16.617	-15.399	1.00	10.67
9375	OG	SER	C	67	-33.928	-17.196	-14.174	1.00	12.25
9377	C	SER	C	67	-35.615	-14.776	-16.497	1.00	11.10
9378	O	SER	C	67	-35.568	-15.383	-17.557	1.00	11.90
9379	N	LYS	C	68	-35.868	-13.476	-16.424	1.00	12.46
9381	CA	LYS	C	68	-36.099	-12.651	-17.605	1.00	12.89
9383	CB	LYS	C	68	-36.218	-11.179	-17.189	1.00	14.02
9386	CG	LYS	C	68	-36.426	-10.209	-18.328	1.00	15.12
9389	CD	LYS	C	68	-36.332	-8.769	-17.850	1.00	15.81
9392	CE	LYS	C	68	-36.418	-7.809	-19.014	1.00	17.58
9395	NZ	LYS	C	68	-36.115	-6.399	-18.628	1.00	18.58
9399	C	LYS	C	68	-35.008	-12.808	-18.676	1.00	12.97
9400	O	LYS	C	68	-35.310	-13.064	-19.844	1.00	12.95
9401	N	GLU	C	69	-33.742	-12.623	-18.303	1.00	13.10
9403	CA	GLU	C	69	-32.678	-12.596	-19.305	1.00	14.14
9405	CB	GLU	C	69	-31.345	-12.082	-18.725	1.00	14.61
9408	CG	BGLU	C	69	-30.505	-11.331	-19.756	0.35	15.94
9409	CG	AGLU	C	69	-30.543	-11.221	-19.693	0.65	18.10
9414	CD	BGLU	C	69	-29.297	-10.613	-19.182	0.35	15.79
9415	CD	AGLU	C	69	-30.963	-9.753	-19.693	0.65	18.95
9416	OE1BGLU	C	69	-28.161	-11.066	-19.436	0.35	14.97	
9417	OE1AGLU	C	69	-32.171	-9.437	-19.823	0.65	20.31	
9418	OE2BGLU	C	69	-29.481	-9.582	-18.503	0.35	17.12	
9419	OE2AGLU	C	69	-30.070	-8.893	-19.530	0.65	23.66	
9420	C	GLU	C	69	-32.500	-13.963	-19.974	1.00	13.34
9421	O	GLU	C	69	-32.335	-14.037	-21.191	1.00	13.45
9422	N	THR	C	70	-32.577	-15.039	-19.202	1.00	12.85
9424	CA	THR	C	70	-32.444	-16.376	-19.782	1.00	12.93
9426	CB	THR	C	70	-32.235	-17.424	-18.683	1.00	13.24
9428	OG1	THR	C	70	-30.969	-17.178	-18.039	1.00	15.98
9430	CG2	THR	C	70	-32.096	-18.819	-19.282	1.00	14.25
9434	C	THR	C	70	-33.657	-16.715	-20.652	1.00	12.07
9435	O	THR	C	70	-33.528	-17.341	-21.700	1.00	11.58
9436	N	LEU	C	71	-34.836	-16.286	-20.231	1.00	11.41
9438	CA	LEU	C	71	-36.038	-16.509	-21.030	1.00	11.28
9440	CB	LEU	C	71	-37.290	-16.022	-20.299	1.00	11.13
9443	CG	LEU	C	71	-37.771	-16.938	-19.175	1.00	11.58
9445	CD1	LEU	C	71	-38.785	-16.187	-18.345	1.00	11.73
9449	CD2	LEU	C	71	-38.351	-18.254	-19.679	1.00	11.28
9453	C	LEU	C	71	-35.929	-15.830	-22.384	1.00	11.10
9454	O	LEU	C	71	-36.337	-16.392	-23.383	1.00	11.02
9455	N	GLN	C	72	-35.356	-14.634	-22.431	1.00	11.25
9457	CA	GLN	C	72	-35.185	-13.959	-23.710	1.00	11.42
9459	CB	GLN	C	72	-34.620	-12.536	-23.520	1.00	11.62

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
9462	CG	GLN	C	72	-34.302	-11.835	-24.834	1.00	12.95
9465	CD	GLN	C	72	-35.524	-11.602	-25.711	1.00	14.15
9466	OE1	GLN	C	72	-35.743	-12.326	-26.701	1.00	18.98
9467	NE2	GLN	C	72	-36.300	-10.584	-25.379	1.00	13.78
9470	C	GLN	C	72	-34.277	-14.783	-24.618	1.00	11.45
9471	O	GLN	C	72	-34.541	-14.900	-25.819	1.00	11.46
9472	N	LYS	C	73	-33.213	-15.364	-24.059	1.00	11.62
9474	CA	LYS	C	73	-32.305	-16.195	-24.843	1.00	12.27
9476	CB	LYS	C	73	-31.047	-16.542	-24.050	1.00	12.53
9479	CG	LYS	C	73	-30.197	-15.326	-23.702	1.00	15.49
9482	CD	LYS	C	73	-29.023	-15.740	-22.829	1.00	19.38
9485	CE	LYS	C	73	-28.051	-14.607	-22.591	1.00	21.70
9488	NZ	LYS	C	73	-26.915	-15.100	-21.778	1.00	25.05
9492	C	LYS	C	73	-33.013	-17.458	-25.336	1.00	11.58
9493	O	LYS	C	73	-32.810	-17.864	-26.475	1.00	11.76
9494	N	VAL	C	74	-33.875	-18.045	-24.501	1.00	11.32
9496	CA	VAL	C	74	-34.642	-19.223	-24.899	1.00	10.74
9498	CB	VAL	C	74	-35.436	-19.812	-23.696	1.00	10.92
9500	CG1	VAL	C	74	-36.476	-20.831	-24.134	1.00	10.72
9504	CG2	VAL	C	74	-34.488	-20.432	-22.699	1.00	10.97
9508	C	VAL	C	74	-35.569	-18.879	-26.063	1.00	10.41
9509	O	VAL	C	74	-35.632	-19.614	-27.045	1.00	10.95
9510	N	VAL	C	75	-36.236	-17.741	-25.968	1.00	10.61
9512	CA	VAL	C	75	-37.153	-17.285	-27.010	1.00	10.51
9514	CB	VAL	C	75	-37.881	-15.991	-26.585	1.00	10.44
9516	CG1	VAL	C	75	-38.982	-16.328	-25.569	1.00	11.03
9520	CG2	VAL	C	75	-38.469	-15.244	-27.769	1.00	11.93
9524	C	VAL	C	75	-36.407	-17.086	-28.325	1.00	10.54
9525	O	VAL	C	75	-36.863	-17.528	-29.362	1.00	10.92
9526	N	SER	C	76	-35.253	-16.435	-28.267	1.00	10.96
9528	CA	SER	C	76	-34.495	-16.165	-29.475	1.00	11.67
9530	CB	SER	C	76	-33.285	-15.290	-29.151	1.00	11.99
9533	OG	SER	C	76	-33.754	-13.994	-28.794	1.00	14.79
9535	C	SER	C	76	-34.077	-17.455	-30.151	1.00	11.70
9536	O	SER	C	76	-34.151	-17.567	-31.372	1.00	12.66
9537	N	HIS	C	77	-33.655	-18.439	-29.364	1.00	11.16
9539	CA	HIS	C	77	-33.272	-19.735	-29.917	1.00	11.51
9541	CB	HIS	C	77	-32.540	-20.580	-28.883	1.00	11.86
9544	CG	HIS	C	77	-31.878	-21.786	-29.468	1.00	13.66
9545	ND1	HIS	C	77	-30.896	-21.694	-30.433	1.00	17.29
9547	CE1	HIS	C	77	-30.496	-22.909	-30.765	1.00	17.57
9549	NE2	HIS	C	77	-31.198	-23.785	-30.071	1.00	17.33
9551	CD2	HIS	C	77	-32.079	-23.107	-29.261	1.00	16.44
9553	C	HIS	C	77	-34.482	-20.489	-30.501	1.00	11.30
9554	O	HIS	C	77	-34.366	-21.157	-31.537	1.00	10.83
9555	N	CYS	C	78	-35.636	-20.391	-29.837	1.00	11.00
9557	CA	CYS	C	78	-36.873	-20.999	-30.342	1.00	11.06
9559	CB	CYS	C	78	-38.040	-20.744	-29.385	1.00	10.77
9562	SG	CYS	C	78	-38.031	-21.772	-27.904	1.00	11.67

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
9563	C	CYS	C	78	-37.208	-20.429	-31.729	1.00	11.12
9564	O	CYS	C	78	-37.577	-21.167	-32.638	1.00	10.85
9565	N	LEU	C	79	-37.045	-19.122	-31.905	1.00	11.29
9567	CA	LEU	C	79	-37.296	-18.516	-33.207	1.00	11.68
9569	CB	LEU	C	79	-37.239	-16.984	-33.133	1.00	11.95
9572	CG	LEU	C	79	-38.341	-16.350	-32.266	1.00	12.31
9574	CD1	LEU	C	79	-39.728	-16.672	-32.783	1.00	13.03
9578	CD2	LEU	C	79	-38.145	-14.845	-32.145	1.00	14.85
9582	C	LEU	C	79	-36.306	-19.067	-34.247	1.00	12.25
9583	O	LEU	C	79	-36.710	-19.412	-35.354	1.00	11.91
9584	N	GLU	C	80	-35.027	-19.187	-33.878	1.00	12.83
9586	CA	GLU	C	80	-34.002	-19.730	-34.783	1.00	13.65
9588	CB	GLU	C	80	-32.614	-19.729	-34.112	1.00	14.43
9591	CG	GLU	C	80	-32.013	-18.372	-33.770	1.00	19.06
9594	CD	GLU	C	80	-30.662	-18.500	-33.065	1.00	23.60
9595	OE1	GLU	C	80	-30.443	-19.482	-32.307	1.00	27.14
9596	OE2	GLU	C	80	-29.804	-17.611	-33.260	1.00	27.59
9597	C	GLU	C	80	-34.328	-21.160	-35.214	1.00	12.95
9598	O	GLU	C	80	-34.103	-21.551	-36.368	1.00	13.12
9599	N	LEU	C	81	-34.861	-21.941	-34.278	1.00	12.08
9601	CA	LEU	C	81	-35.196	-23.338	-34.514	1.00	11.72
9603	CB	LEU	C	81	-35.397	-24.074	-33.177	1.00	12.04
9606	CG	LEU	C	81	-34.149	-24.299	-32.334	1.00	12.68
9608	CD1	LEU	C	81	-34.523	-24.806	-30.955	1.00	13.46
9612	CD2	LEU	C	81	-33.209	-25.277	-33.025	1.00	13.08
9616	C	LEU	C	81	-36.441	-23.546	-35.371	1.00	11.61
9617	O	LEU	C	81	-36.663	-24.655	-35.835	1.00	12.71
9618	N	GLY	C	82	-37.245	-22.497	-35.557	1.00	11.32
9620	CA	GLY	C	82	-38.409	-22.544	-36.424	1.00	11.36
9623	C	GLY	C	82	-39.765	-22.453	-35.753	1.00	11.12
9624	O	GLY	C	82	-40.774	-22.818	-36.371	1.00	10.81
9625	N	ALA	C	83	-39.818	-21.944	-34.519	1.00	10.96
9627	CA	ALA	C	83	-41.103	-21.719	-33.859	1.00	10.61
9629	CB	ALA	C	83	-40.924	-21.092	-32.487	1.00	10.78
9633	C	ALA	C	83	-41.982	-20.835	-34.721	1.00	10.78
9634	O	ALA	C	83	-41.506	-19.896	-35.346	1.00	10.50
9635	N	ALA	C	84	-43.263	-21.172	-34.790	1.00	10.06
9637	CA	ALA	C	84	-44.223	-20.308	-35.468	1.00	10.19
9639	CB	ALA	C	84	-45.597	-20.904	-35.412	1.00	10.24
9643	C	ALA	C	84	-44.217	-18.919	-34.855	1.00	9.82
9644	O	ALA	C	84	-44.379	-17.920	-35.559	1.00	10.50
9645	N	SER	C	85	-44.076	-18.891	-33.530	1.00	10.08
9647	CA	SER	C	85	-43.855	-17.678	-32.750	1.00	10.63
9649	CB	SER	C	85	-45.127	-16.846	-32.601	1.00	11.36
9652	OG	SER	C	85	-46.115	-17.487	-31.792	1.00	13.29
9654	C	SER	C	85	-43.350	-18.100	-31.370	1.00	10.36
9655	O	SER	C	85	-43.522	-19.246	-30.957	1.00	10.45
9656	N	ALA	C	86	-42.710	-17.174	-30.678	1.00	10.36
9658	CA	ALA	C	86	-42.191	-17.445	-29.341	1.00	10.21

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
9660	CB	ALA	C	86	-40.825	-18.087	-29.410	1.00	10.25
9664	C	ALA	C	86	-42.134	-16.147	-28.534	1.00	10.14
9665	O	ALA	C	86	-41.638	-15.136	-29.009	1.00	9.59
9666	N	HIS	C	87	-42.673	-16.194	-27.317	1.00	9.93
9668	CA	HIS	C	87	-42.656	-15.079	-26.373	1.00	10.62
9670	CB	HIS	C	87	-44.001	-14.352	-26.350	1.00	10.72
9673	CG	HIS	C	87	-44.411	-13.831	-27.683	1.00	13.45
9674	ND1	HIS	C	87	-43.930	-12.650	-28.205	1.00	16.20
9676	CE1	HIS	C	87	-44.431	-12.471	-29.413	1.00	14.34
9678	NE2	HIS	C	87	-45.224	-13.486	-29.688	1.00	17.69
9680	CD2	HIS	C	87	-45.229	-14.352	-28.622	1.00	13.92
9682	C	HIS	C	87	-42.390	-15.627	-24.982	1.00	10.03
9683	O	HIS	C	87	-42.629	-16.804	-24.715	1.00	10.03
9684	N	TYR	C	88	-41.875	-14.767	-24.115	1.00	10.50
9686	CA	TYR	C	88	-41.756	-15.081	-22.699	1.00	10.47
9688	CB	TYR	C	88	-40.287	-15.144	-22.243	1.00	10.56
9691	CG	TYR	C	88	-39.648	-13.793	-22.020	1.00	10.93
9692	CD1	TYR	C	88	-39.806	-13.116	-20.815	1.00	12.28
9694	CE1	TYR	C	88	-39.242	-11.861	-20.618	1.00	13.12
9696	CZ	TYR	C	88	-38.508	-11.284	-21.623	1.00	13.73
9697	OH	TYR	C	88	-37.944	-10.033	-21.437	1.00	15.02
9699	CE2	TYR	C	88	-38.324	-11.948	-22.819	1.00	11.86
9701	CD2	TYR	C	88	-38.904	-13.189	-23.016	1.00	12.50
9703	C	TYR	C	88	-42.518	-14.074	-21.872	1.00	10.92
9704	O	TYR	C	88	-42.740	-12.927	-22.281	1.00	10.95
9705	N	ILE	C	89	-42.908	-14.526	-20.687	1.00	10.32
9707	CA	ILE	C	89	-43.421	-13.662	-19.633	1.00	11.13
9709	CB	ILE	C	89	-44.951	-13.786	-19.529	1.00	11.03
9711	CG1	ILE	C	89	-45.632	-13.369	-20.845	1.00	12.20
9714	CD1	ILE	C	89	-47.114	-13.657	-20.893	1.00	13.25
9718	CG2	ILE	C	89	-45.468	-12.927	-18.386	1.00	11.68
9722	C	ILE	C	89	-42.757	-14.138	-18.350	1.00	11.21
9723	O	ILE	C	89	-42.842	-15.311	-18.011	1.00	11.66
9724	N	ALA	C	90	-42.073	-13.235	-17.653	1.00	11.07
9726	CA	ALA	C	90	-41.313	-13.593	-16.456	1.00	11.45
9728	CB	ALA	C	90	-40.004	-12.836	-16.395	1.00	11.59
9732	C	ALA	C	90	-42.135	-13.312	-15.217	1.00	11.90
9733	O	ALA	C	90	-42.825	-12.290	-15.123	1.00	12.14
9734	N	GLY	C	91	-42.059	-14.226	-14.263	1.00	11.45
9736	CA	GLY	C	91	-42.694	-14.025	-12.977	1.00	11.43
9739	C	GLY	C	91	-42.545	-15.235	-12.092	1.00	11.15
9740	O	GLY	C	91	-42.062	-16.293	-12.521	1.00	11.42
9741	N	THR	C	92	-42.950	-15.074	-10.839	1.00	10.96
9743	CA	THR	C	92	-42.914	-16.186	-9.899	1.00	10.73
9745	CB	THR	C	92	-42.310	-15.787	-8.540	1.00	11.32
9747	OG1	THR	C	92	-42.439	-16.897	-7.639	1.00	11.27
9749	CG2	THR	C	92	-43.089	-14.648	-7.878	1.00	12.24
9753	C	THR	C	92	-44.295	-16.788	-9.710	1.00	10.61
9754	O	THR	C	92	-45.278	-16.082	-9.522	1.00	10.35

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
9755	N	MET	C	93	-44.341	-18.116	-9.747	1.00	10.55
9757	CA	MET	C	93	-45.568	-18.869	-9.598	1.00	11.21
9759	CB	MET	C	93	-45.447	-20.230	-10.301	1.00	10.93
9762	CG	MET	C	93	-45.403	-20.125	-11.808	1.00	10.86
9765	SD	MET	C	93	-46.979	-19.547	-12.465	1.00	12.03
9766	CE	MET	C	93	-46.585	-19.480	-14.210	1.00	13.53
9770	C	MET	C	93	-45.967	-19.024	-8.127	1.00	12.30
9771	O	MET	C	93	-46.930	-19.716	-7.822	1.00	13.81
9772	N	GLU	C	94	-45.228	-18.372	-7.237	1.00	12.60
9774	CA	GLU	C	94	-45.681	-18.142	-5.855	1.00	13.42
9776	CB	GLU	C	94	-44.561	-17.541	-4.993	1.00	14.22
9779	CG	GLU	C	94	-43.221	-18.264	-4.964	1.00	17.38
9782	CD	GLU	C	94	-42.097	-17.360	-4.450	1.00	21.80
9783	OE1	GLU	C	94	-41.471	-16.601	-5.245	1.00	22.26
9784	OE2	GLU	C	94	-41.854	-17.393	-3.222	1.00	25.46
9785	C	GLU	C	94	-46.849	-17.144	-5.849	1.00	13.33
9786	O	GLU	C	94	-47.639	-17.106	-4.912	1.00	14.06
9787	N	ASP	C	95	-46.932	-16.327	-6.891	1.00	13.30
9789	CA	ASP	C	95	-47.931	-15.264	-7.004	1.00	13.37
9791	CB	ASP	C	95	-47.258	-14.040	-7.621	1.00	13.79
9794	CG	ASP	C	95	-48.166	-12.843	-7.732	1.00	15.27
9795	OD1	ASP	C	95	-49.405	-12.981	-7.673	1.00	16.12
9796	OD2	ASP	C	95	-47.702	-11.698	-7.877	1.00	18.74
9797	C	ASP	C	95	-49.099	-15.764	-7.850	1.00	13.24
9798	O	ASP	C	95	-48.979	-15.902	-9.071	1.00	12.96
9799	N	MET	C	96	-50.220	-16.067	-7.204	1.00	13.39
9801	CA	MET	C	96	-51.362	-16.660	-7.910	1.00	13.65
9803	CB	MET	C	96	-52.406	-17.203	-6.924	1.00	14.47
9806	CG	MET	C	96	-51.901	-18.298	-5.979	1.00	15.32
9809	SD	MET	C	96	-51.228	-19.753	-6.817	1.00	17.26
9810	CE	MET	C	96	-49.705	-20.017	-5.948	1.00	16.93
9814	C	MET	C	96	-52.009	-15.661	-8.881	1.00	13.50
9815	O	MET	C	96	-52.616	-16.058	-9.876	1.00	13.25
9816	N	THR	C	97	-51.907	-14.369	-8.593	1.00	13.11
9818	CA	THR	C	97	-52.396	-13.370	-9.541	1.00	13.69
9820	CB	THR	C	97	-52.387	-11.981	-8.926	1.00	14.13
9822	OG1	THR	C	97	-53.233	-11.993	-7.776	1.00	15.04
9824	CG2	THR	C	97	-53.020	-10.965	-9.874	1.00	15.45
9828	C	THR	C	97	-51.558	-13.395	-10.801	1.00	13.08
9829	O	THR	C	97	-52.093	-13.319	-11.903	1.00	13.47
9830	N	PHE	C	98	-50.243	-13.501	-10.643	1.00	12.85
9832	CA	PHE	C	98	-49.366	-13.620	-11.806	1.00	12.31
9834	CB	PHE	C	98	-47.886	-13.719	-11.427	1.00	12.66
9837	CG	PHE	C	98	-47.022	-14.112	-12.594	1.00	12.26
9838	CD1	PHE	C	98	-46.781	-13.204	-13.609	1.00	13.75
9840	CE1	PHE	C	98	-46.035	-13.558	-14.720	1.00	13.31
9842	CZ	PHE	C	98	-45.540	-14.841	-14.838	1.00	13.65
9844	CE2	PHE	C	98	-45.787	-15.767	-13.842	1.00	12.88
9846	CD2	PHE	C	98	-46.537	-15.399	-12.723	1.00	14.35

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
9848	C	PHE	C	98	-49.768	-14.832	-12.636	1.00	12.27
9849	O	PHE	C	98	-49.851	-14.755	-13.857	1.00	12.04
9850	N	ALA	C	99	-50.004	-15.962	-11.980	1.00	11.95
9852	CA	ALA	C	99	-50.390	-17.180	-12.690	1.00	12.34
9854	CB	ALA	C	99	-50.588	-18.316	-11.718	1.00	12.81
9858	C	ALA	C	99	-51.640	-16.966	-13.547	1.00	12.68
9859	O	ALA	C	99	-51.650	-17.293	-14.736	1.00	12.01
9860	N	GLU	C	100	-52.682	-16.394	-12.946	1.00	13.19
9862	CA	GLU	C	100	-53.921	-16.063	-13.656	1.00	14.53
9864	CB	GLU	C	100	-54.874	-15.307	-12.737	1.00	15.69
9867	CG	GLU	C	100	-55.456	-16.092	-11.593	1.00	19.04
9870	CD	GLU	C	100	-56.334	-15.220	-10.702	1.00	23.74
9871	OE1	GLU	C	100	-57.237	-15.772	-10.055	1.00	27.43
9872	OE2	GLU	C	100	-56.119	-13.980	-10.640	1.00	27.05
9873	C	GLU	C	100	-53.679	-15.160	-14.858	1.00	13.87
9874	O	GLU	C	100	-54.128	-15.445	-15.982	1.00	14.88
9875	N	GLN	C	101	-52.963	-14.070	-14.615	1.00	13.12
9877	CA	GLN	C	101	-52.725	-13.058	-15.636	1.00	13.26
9879	CB	GLN	C	101	-52.100	-11.804	-15.022	1.00	13.37
9882	CG	GLN	C	101	-53.044	-11.055	-14.068	1.00	16.52
9885	CD	GLN	C	101	-52.430	-9.780	-13.512	1.00	19.64
9886	OE1	GLN	C	101	-51.244	-9.521	-13.701	1.00	23.65
9887	NE2	GLN	C	101	-53.238	-8.984	-12.824	1.00	22.00
9890	C	GLN	C	101	-51.833	-13.595	-16.748	1.00	12.72
9891	O	GLN	C	101	-51.995	-13.233	-17.918	1.00	13.99
9892	N	PHE	C	102	-50.905	-14.474	-16.387	1.00	11.29
9894	CA	PHE	C	102	-49.990	-15.077	-17.344	1.00	10.48
9896	CB	PHE	C	102	-49.000	-16.013	-16.631	1.00	10.52
9899	CG	PHE	C	102	-48.303	-16.931	-17.562	1.00	10.45
9900	CD1	PHE	C	102	-47.356	-16.433	-18.424	1.00	9.23
9902	CE1	PHE	C	102	-46.735	-17.262	-19.353	1.00	11.22
9904	CZ	PHE	C	102	-47.080	-18.593	-19.416	1.00	10.65
9906	CE2	PHE	C	102	-48.035	-19.088	-18.559	1.00	11.41
9908	CD2	PHE	C	102	-48.645	-18.268	-17.645	1.00	11.66
9910	C	PHE	C	102	-50.744	-15.854	-18.412	1.00	10.11
9911	O	PHE	C	102	-50.466	-15.721	-19.608	1.00	9.83
9912	N	VAL	C	103	-51.688	-16.682	-17.995	1.00	10.41
9914	CA	VAL	C	103	-52.415	-17.509	-18.952	1.00	10.86
9916	CB	VAL	C	103	-53.333	-18.534	-18.243	1.00	10.82
9918	CG1	VAL	C	103	-54.222	-19.259	-19.238	1.00	12.10
9922	CG2	VAL	C	103	-52.492	-19.540	-17.473	1.00	11.88
9926	C	VAL	C	103	-53.237	-16.642	-19.901	1.00	10.74
9927	O	VAL	C	103	-53.276	-16.906	-21.103	1.00	10.87
9928	N	ALA	C	104	-53.863	-15.595	-19.369	1.00	11.18
9930	CA	ALA	C	104	-54.683	-14.704	-20.182	1.00	11.65
9932	CB	ALA	C	104	-55.394	-13.679	-19.325	1.00	11.89
9936	C	ALA	C	104	-53.810	-14.025	-21.227	1.00	11.62
9937	O	ALA	C	104	-54.191	-13.938	-22.392	1.00	12.71
9938	N	GLN	C	105	-52.629	-13.574	-20.823	1.00	11.78

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
9940	CA	GLN	C	105	-51.735	-12.903	-21.774	1.00	11.48
9942	CB	GLN	C	105	-50.637	-12.130	-21.054	1.00	11.87
9945	CG	GLN	C	105	-49.714	-11.329	-21.976	1.00	13.85
9948	CD	GLN	C	105	-50.388	-10.160	-22.707	1.00	16.20
9949	OE1	GLN	C	105	-51.535	-9.790	-22.432	1.00	17.95
9950	NE2	GLN	C	105	-49.653	-9.569	-23.634	1.00	19.10
9953	C	GLN	C	105	-51.150	-13.879	-22.775	1.00	11.40
9954	O	GLN	C	105	-51.061	-13.562	-23.957	1.00	11.34
9955	N	ALA	C	106	-50.770	-15.074	-22.328	1.00	10.66
9957	CA	ALA	C	106	-50.238	-16.081	-23.245	1.00	11.05
9959	CB	ALA	C	106	-49.813	-17.320	-22.494	1.00	10.68
9963	C	ALA	C	106	-51.264	-16.434	-24.325	1.00	10.96
9964	O	ALA	C	106	-50.916	-16.580	-25.503	1.00	11.06
9965	N	GLY	C	107	-52.527	-16.541	-23.927	1.00	11.32
9967	CA	GLY	C	107	-53.619	-16.825	-24.842	1.00	11.85
9970	C	GLY	C	107	-53.770	-15.737	-25.885	1.00	12.19
9971	O	GLY	C	107	-54.005	-16.027	-27.057	1.00	12.87
9972	N	LYS	C	108	-53.603	-14.483	-25.472	1.00	12.13
9974	CA	LYS	C	108	-53.690	-13.360	-26.405	1.00	11.90
9976	CB	LYS	C	108	-53.778	-12.041	-25.652	1.00	12.00
9979	CG	LYS	C	108	-55.099	-11.828	-24.978	1.00	13.13
9982	CD	LYS	C	108	-55.061	-10.604	-24.114	1.00	16.74
9985	CE	LYS	C	108	-56.325	-10.440	-23.309	1.00	18.83
9988	NZ	LYS	C	108	-56.137	-9.316	-22.351	1.00	20.85
9992	C	LYS	C	108	-52.508	-13.339	-27.360	1.00	11.60
9993	O	LYS	C	108	-52.648	-12.965	-28.535	1.00	11.38
9994	N	LEU	C	109	-51.333	-13.712	-26.859	1.00	11.21
9996	CA	LEU	C	109	-50.136	-13.743	-27.690	1.00	11.45
9998	CB	LEU	C	109	-48.892	-14.021	-26.846	1.00	10.99
10001	CG	LEU	C	109	-48.435	-12.832	-26.001	1.00	11.40
10003	CD1	LEU	C	109	-47.465	-13.265	-24.921	1.00	11.64
10007	CD2	LEU	C	109	-47.809	-11.750	-26.878	1.00	11.41
10011	C	LEU	C	109	-50.232	-14.771	-28.805	1.00	11.60
10012	O	LEU	C	109	-49.680	-14.563	-29.891	1.00	13.02
10013	N	MET	C	110	-50.913	-15.887	-28.546	1.00	11.68
10015	CA	MET	C	110	-51.011	-16.982	-29.514	1.00	11.43
10017	CB	MET	C	110	-50.707	-18.317	-28.826	1.00	11.22
10020	CG	MET	C	110	-49.320	-18.358	-28.203	1.00	11.11
10023	SD	MET	C	110	-48.806	-19.991	-27.682	1.00	11.22
10024	CE	MET	C	110	-49.733	-20.156	-26.217	1.00	11.83
10028	C	MET	C	110	-52.367	-17.092	-30.216	1.00	11.79
10029	O	MET	C	110	-52.489	-17.833	-31.195	1.00	12.14
10030	N	GLY	C	111	-53.371	-16.364	-29.742	1.00	11.94
10032	CA	GLY	C	111	-54.726	-16.503	-30.262	1.00	12.21
10035	C	GLY	C	111	-55.390	-17.812	-29.890	1.00	12.63
10036	O	GLY	C	111	-56.146	-18.384	-30.678	1.00	13.55
10037	N	GLY	C	112	-55.132	-18.275	-28.674	1.00	11.86
10039	CA	GLY	C	112	-55.694	-19.522	-28.193	1.00	11.30
10042	C	GLY	C	112	-54.677	-20.368	-27.462	1.00	10.88



# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
10043	O	GLY	C	112	-53.559	-19.938	-27.206	1.00	10.98
10044	N	LEU	C	113	-55.078	-21.592	-27.141	1.00	10.04
10046	CA	LEU	C	113	-54.238	-22.519	-26.407	1.00	10.43
10048	CB	LEU	C	113	-54.342	-22.250	-24.897	1.00	10.59
10051	CG	LEU	C	113	-53.380	-23.040	-24.013	1.00	10.78
10053	CD1	LEU	C	113	-51.932	-22.619	-24.262	1.00	11.54
10057	CD2	LEU	C	113	-53.724	-22.851	-22.550	1.00	11.09
10061	C	LEU	C	113	-54.647	-23.956	-26.700	1.00	10.54
10062	O	LEU	C	113	-55.813	-24.326	-26.520	1.00	11.26
10063	N	ASP	C	114	-53.680	-24.756	-27.147	1.00	10.61
10065	CA	ASP	C	114	-53.872	-26.176	-27.405	1.00	10.85
10067	CB	ASP	C	114	-53.228	-26.563	-28.736	1.00	10.89
10070	CG	ASP	C	114	-53.853	-25.860	-29.906	1.00	12.73
10071	OD1	ASP	C	114	-55.052	-26.117	-30.193	1.00	15.70
10072	OD2	ASP	C	114	-53.218	-25.053	-30.618	1.00	12.90
10073	C	ASP	C	114	-53.288	-27.076	-26.331	1.00	10.75
10074	O	ASP	C	114	-53.790	-28.164	-26.118	1.00	11.16
10075	N	MET	C	115	-52.213	-26.643	-25.679	1.00	10.45
10077	CA	MET	C	115	-51.507	-27.489	-24.719	1.00	10.74
10079	CB	MET	C	115	-50.417	-28.305	-25.402	1.00	11.23
10082	CG	MET	C	115	-49.751	-29.324	-24.485	1.00	11.94
10085	SD	MET	C	115	-48.491	-30.360	-25.284	1.00	15.8
10086	CE	MET	C	115	-49.523	-31.663	-25.938	1.00	17.69
10090	C	MET	C	115	-50.894	-26.643	-23.621	1.00	10.76
10091	O	MET	C	115	-50.205	-25.668	-23.891	1.00	10.73
10092	N	LEU	C	116	-51.123	-27.059	-22.386	1.00	10.32
10094	CA	LEU	C	116	-50.601	-26.400	-21.211	1.00	10.64
10096	CB	LEU	C	116	-51.751	-26.087	-20.268	1.00	10.39
10099	CG	LEU	C	116	-51.387	-25.485	-18.926	1.00	11.20
10101	CD1	LEU	C	116	-50.827	-24.088	-19.093	1.00	11.89
10105	CD2	LEU	C	116	-52.607	-25.480	-18.048	1.00	11.84
10109	C	LEU	C	116	-49.627	-27.378	-20.549	1.00	10.31
10110	O	LEU	C	116	-50.043	-28.406	-20.018	1.00	11.38
10111	N	ILE	C	117	-48.337	-27.067	-20.586	1.00	9.60
10113	CA	ILE	C	117	-47.328	-27.923	-19.980	1.00	9.58
10115	CB	ILE	C	117	-46.127	-28.149	-20.926	1.00	9.64
10117	CG1	ILE	C	117	-46.594	-28.770	-22.248	1.00	10.29
10120	CD1	ILE	C	117	-45.487	-29.065	-23.271	1.00	11.58
10124	CG2	ILE	C	117	-45.104	-29.054	-20.246	1.00	10.50
10128	C	ILE	C	117	-46.871	-27.285	-18.681	1.00	9.81
10129	O	ILE	C	117	-46.233	-26.227	-18.661	1.00	9.40
10130	N	LEU	C	118	-47.254	-27.933	-17.586	1.00	9.04
10132	CA	LEU	C	118	-46.979	-27.482	-16.242	1.00	9.06
10134	CB	LEU	C	118	-48.214	-27.724	-15.382	1.00	9.37
10137	CG	LEU	C	118	-49.481	-27.078	-15.926	1.00	10.39
10139	CD1	LEU	C	118	-50.675	-27.486	-15.098	1.00	11.51
10143	CD2	LEU	C	118	-49.352	-25.555	-15.952	1.00	11.76
10147	C	LEU	C	118	-45.768	-28.237	-15.701	1.00	9.53
10148	O	LEU	C	118	-45.832	-29.428	-15.442	1.00	9.57

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
10149	N	ASN	C	119	-44.666	-27.520	-15.525	1.00	9.00
10151	CA	ASN	C	119	-43.383	-28.159	-15.276	1.00	9.50
10153	CB	ASN	C	119	-42.627	-28.174	-16.615	1.00	9.91
10156	CG	ASN	C	119	-41.147	-28.419	-16.477	1.00	10.58
10157	OD1	ASN	C	119	-40.338	-27.457	-16.459	1.00	13.51
10158	ND2	ASN	C	119	-40.762	-29.673	-16.405	1.00	7.46
10161	C	ASN	C	119	-42.559	-27.535	-14.141	1.00	9.42
10162	O	ASN	C	119	-41.707	-28.196	-13.562	1.00	10.26
10163	N	HIS	C	120	-42.788	-26.263	-13.826	1.00	9.55
10165	CA	HIS	C	120	-42.003	-25.586	-12.805	1.00	9.10
10167	CB	HIS	C	120	-42.412	-24.123	-12.710	1.00	9.31
10170	CG	HIS	C	120	-43.833	-23.919	-12.303	1.00	10.66
10171	ND1	HIS	C	120	-44.863	-23.853	-13.213	1.00	11.17
10173	CE1	HIS	C	120	-45.999	-23.655	-12.569	1.00	11.17
10175	NE2	HIS	C	120	-45.747	-23.617	-11.272	1.00	10.80
10177	CD2	HIS	C	120	-44.401	-23.797	-11.079	1.00	10.69
10179	C	HIS	C	120	-42.138	-26.207	-11.405	1.00	9.58
10180	O	HIS	C	120	-43.158	-26.804	-11.056	1.00	9.29
10181	N	ILE	C	121	-41.088	-26.033	-10.621	1.00	9.72
10183	CA	ILE	C	121	-41.097	-26.336	-9.192	1.00	9.66
10185	CB	ILE	C	121	-40.481	-27.730	-8.871	1.00	9.69
10187	CG1	ILE	C	121	-39.077	-27.851	-9.465	1.00	11.66
10190	CD1	ILE	C	121	-38.329	-29.099	-8.981	1.00	13.48
10194	CG2	ILE	C	121	-41.391	-28.830	-9.342	1.00	9.04
10198	C	ILE	C	121	-40.301	-25.279	-8.465	1.00	10.04
10199	O	ILE	C	121	-39.454	-24.598	-9.060	1.00	10.46
10200	N	THR	C	122	-40.550	-25.164	-7.175	1.00	9.95
10202	CA	THR	C	122	-39.726	-24.308	-6.330	1.00	11.42
10204	CB	THR	C	122	-40.517	-23.903	-5.087	1.00	11.76
10206	OG1	THR	C	122	-39.838	-22.832	-4.412	1.00	11.76
10208	CG2	THR	C	122	-40.604	-25.026	-4.071	1.00	12.14
10212	C	THR	C	122	-38.423	-25.016	-5.963	1.00	12.88
10213	O	THR	C	122	-38.339	-26.239	-6.024	1.00	13.41
10214	N	ASN	C	123	-37.407	-24.248	-5.571	1.00	14.51
10216	CA	ASN	C	123	-36.109	-24.828	-5.234	1.00	16.88
10218	CB	ASN	C	123	-35.170	-23.770	-4.665	1.00	17.35
10221	CG	ASN	C	123	-33.804	-24.335	-4.328	1.00	21.50
10222	OD1	ASN	C	123	-33.467	-24.518	-3.161	1.00	27.20
10223	ND2	ASN	C	123	-33.022	-24.649	-5.358	1.00	26.81
10226	C	ASN	C	123	-36.246	-25.957	-4.227	1.00	16.95
10227	O	ASN	C	123	-36.828	-25.777	-3.174	1.00	16.58
10228	N	THR	C	124	-35.690	-27.111	-4.587	1.00	18.02
10230	CA	THR	C	124	-35.783	-28.339	-3.818	1.00	18.77
10232	CB	THR	C	124	-36.777	-29.282	-4.513	1.00	19.02
10234	OG1	THR	C	124	-38.070	-28.665	-4.514	1.00	20.80
10236	CG2	THR	C	124	-36.965	-30.563	-3.727	1.00	18.30
10240	C	THR	C	124	-34.404	-28.988	-3.780	1.00	19.65
10241	O	THR	C	124	-33.784	-29.168	-4.827	1.00	20.22
10242	N	SER	C	125	-33.924	-29.297	-2.582	1.00	19.97

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
10244	CA	SER	C	125	-32.731	-30.127	-2.417	1.00	20.51
10246	CB	SER	C	125	-31.539	-29.260	-2.003	1.00	20.74
10249	OG	SER	C	125	-31.800	-28.570	-0.794	1.00	22.53
10251	C	SER	C	125	-32.992	-31.250	-1.401	1.00	20.25
10252	O	SER	C	125	-34.048	-31.302	-0.754	1.00	20.81
10253	N	LEU	C	126	-32.039	-32.165	-1.273	1.00	19.17
10255	CA	LEU	C	126	-32.186	-33.295	-0.366	1.00	18.81
10257	CB	LEU	C	126	-31.322	-34.470	-0.829	1.00	18.81
10260	CG	LEU	C	126	-31.601	-34.931	-2.265	1.00	19.10
10262	CD1	LEU	C	126	-30.680	-36.082	-2.646	1.00	20.60
10266	CD2	LEU	C	126	-33.052	-35.336	-2.424	1.00	19.16
10270	C	LEU	C	126	-31.826	-32.883	1.060	1.00	18.46
10271	O	LEU	C	126	-30.671	-32.562	1.349	1.00	18.15
10272	N	ASN	C	127	-32.826	-32.872	1.940	1.00	17.75
10274	CA	ASN	C	127	-32.619	-32.609	3.365	1.00	18.29
10276	CB	BASN	C	127	-32.658	-31.100	3.652	0.35	18.44
10277	CB	AASN	C	127	-32.661	-31.108	3.646	0.65	19.02
10282	CG	BASN	C	127	-31.963	-30.268	2.578	0.35	18.55
10283	CG	AASN	C	127	-31.294	-30.446	3.534	0.65	20.64
10284	OD1	BASN	C	127	-32.609	-29.734	1.674	0.35	19.74
10285	OD1	AASN	C	127	-30.300	-30.932	4.084	0.65	24.10
10286	ND2	BASN	C	127	-30.639	-30.163	2.672	0.35	18.96
10287	ND2	AASN	C	127	-31.244	-29.322	2.824	0.65	22.89
10292	C	ASN	C	127	-33.688	-33.311	4.191	1.00	18.03
10293	O	ASN	C	127	-34.808	-33.488	3.729	1.00	17.44
10294	N	LEU	C	128	-33.358	-33.681	5.422	1.00	18.13
10296	CA	LEU	C	128	-34.354	-34.195	6.349	1.00	18.63
10298	CB	LEU	C	128	-33.708	-34.668	7.650	1.00	19.11
10301	CG	LEU	C	128	-32.840	-35.931	7.596	1.00	19.91
10303	CD1	LEU	C	128	-31.916	-36.009	8.796	1.00	20.83
10307	CD2	LEU	C	128	-33.698	-37.177	7.532	1.00	20.96
10311	C	LEU	C	128	-35.362	-33.091	6.658	1.00	18.94
10312	O	LEU	C	128	-35.025	-31.901	6.631	1.00	19.50
10313	N	PHE	C	129	-36.599	-33.492	6.924	1.00	18.66
10315	CA	PHE	C	129	-37.621	-32.590	7.418	1.00	19.13
10317	CB	PHE	C	129	-39.020	-33.154	7.231	1.00	18.55
10320	CG	PHE	C	129	-40.091	-32.242	7.746	1.00	16.44
10321	CD1	PHE	C	129	-40.433	-31.107	7.042	1.00	15.38
10323	CE1	PHE	C	129	-41.409	-30.244	7.524	1.00	14.43
10325	CZ	PHE	C	129	-42.031	-30.511	8.710	1.00	14.56
10327	CE2	PHE	C	129	-41.698	-31.641	9.430	1.00	15.64
10329	CD2	PHE	C	129	-40.720	-32.492	8.954	1.00	16.18
10331	C	PHE	C	129	-37.421	-32.344	8.909	1.00	20.90
10332	O	PHE	C	129	-37.716	-33.215	9.745	1.00	21.20
10333	N	HIS	C	130	-36.908	-31.166	9.224	1.00	22.26
10335	CA	HIS	C	130	-36.928	-30.639	10.579	1.00	23.53
10337	CB	HIS	C	130	-35.506	-30.509	11.114	1.00	24.17
10340	CG	HIS	C	130	-34.889	-31.816	11.513	1.00	27.59
10341	ND1	HIS	C	130	-34.203	-32.620	10.626	1.00	31.35

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
10343	CE1	HIS	C	130	-33.768	-33.697	11.256	1.00	31.35
10345	NE2	HIS	C	130	-34.154	-33.627	12.516	1.00	31.40
10347	CD2	HIS	C	130	-34.856	-32.460	12.703	1.00	30.03
10349	C	HIS	C	130	-37.641	-29.286	10.619	1.00	23.20
10350	O	HIS	C	130	-37.050	-28.240	10.333	1.00	22.94
10351	N	ASP	C	131	-38.927	-29.336	10.942	1.00	22.72
10353	CA	ASP	C	131	-39.711	-28.173	11.365	1.00	23.04
10355	CB	ASP	C	131	-39.154	-27.584	12.700	1.00	23.56
10358	CG	ASP	C	131	-38.313	-26.297	12.535	1.00	25.77
10359	OD1	ASP	C	131	-37.727	-26.031	11.457	1.00	30.38
10360	OD2	ASP	C	131	-38.157	-25.480	13.476	1.00	29.41
10361	C	ASP	C	131	-39.951	-27.110	10.282	1.00	21.78
10362	O	ASP	C	131	-40.475	-26.042	10.576	1.00	22.74
10363	N	ASP	C	132	-39.619	-27.420	9.030	1.00	20.50
10365	CA	ASP	C	132	-39.647	-26.410	7.975	1.00	19.51
10367	CB	ASP	C	132	-38.555	-26.664	6.928	1.00	20.02
10370	CG	ASP	C	132	-38.201	-25.411	6.141	1.00	20.05
10371	OD1	ASP	C	132	-38.958	-24.421	6.200	1.00	20.20
10372	OD2	ASP	C	132	-37.161	-25.308	5.455	1.00	22.26
10373	C	ASP	C	132	-41.022	-26.306	7.320	1.00	18.47
10374	O	ASP	C	132	-41.199	-26.625	6.142	1.00	17.67
10375	N	ILE	C	133	-41.982	-25.809	8.090	1.00	17.52
10377	CA	ILE	C	133	-43.346	-25.639	7.611	1.00	17.21
10379	CB	ILE	C	133	-44.276	-25.219	8.770	1.00	17.52
10381	CG1	ILE	C	133	-44.299	-26.306	9.862	1.00	19.82
10384	CD1	ILE	C	133	-44.714	-25.806	11.232	1.00	22.45
10388	CG2	ILE	C	133	-45.690	-24.974	8.274	1.00	17.69
10392	C	ILE	C	133	-43.373	-24.615	6.465	1.00	16.32
10393	O	ILE	C	133	-44.190	-24.713	5.562	1.00	15.00
10394	N	HIS	C	134	-42.459	-23.648	6.486	1.00	15.88
10396	CA	HIS	C	134	-42.390	-22.654	5.410	1.00	16.32
10398	CB	BHIS	C	134	-41.380	-21.548	5.745	0.35	16.05
10399	CB	AHIS	C	134	-41.309	-21.599	5.707	0.65	16.79
10404	CG	BHIS	C	134	-41.828	-20.645	6.858	0.35	16.23
10405	CG	AHIS	C	134	-40.939	-20.751	4.527	0.65	20.03
10406	ND1	BHIS	C	134	-43.111	-20.660	7.362	0.35	16.25
10407	ND1	AHIS	C	134	-39.866	-21.037	3.709	0.65	23.89
10410	CE1	BHIS	C	134	-43.214	-19.768	8.331	0.35	16.83
10411	CE1	AHIS	C	134	-39.785	-20.126	2.755	0.65	23.82
10414	NE2	BHIS	C	134	-42.046	-19.169	8.471	0.35	16.98
10415	NE2	AHIS	C	134	-40.772	-19.264	2.919	0.65	23.25
10418	CD2	BHIS	C	134	-41.162	-19.699	7.562	0.35	16.68
10419	CD2	AHIS	C	134	-41.504	-19.628	4.024	0.65	23.08
10422	C	HIS	C	134	-42.103	-23.318	4.059	1.00	15.27
10423	O	HIS	C	134	-42.728	-22.958	3.064	1.00	14.85
10424	N	HIS	C	135	-41.178	-24.280	4.024	1.00	14.87
10426	CA	HIS	C	135	-40.857	-25.012	2.789	1.00	14.49
10428	CB	HIS	C	135	-39.597	-25.879	2.944	1.00	15.13
10431	CG	HIS	C	135	-39.206	-26.589	1.685	1.00	15.71

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
10432	ND1	HIS	C	135	-39.121	-27.961	1.582	1.00	18.56
10434	CE1	HIS	C	135	-38.769	-28.286	0.350	1.00	17.75
10436	NE2	HIS	C	135	-38.621	-27.175	-0.347	1.00	18.30
10438	CD2	HIS	C	135	-38.887	-26.103	0.464	1.00	15.10
10440	C	HIS	C	135	-42.007	-25.906	2.363	1.00	13.90
10441	O	HIS	C	135	-42.263	-26.077	1.172	1.00	13.64
10442	N	VAL	C	136	-42.713	-26.481	3.332	1.00	12.43
10444	CA	VAL	C	136	-43.875	-27.298	3.006	1.00	12.03
10446	CB	VAL	C	136	-44.471	-27.987	4.247	1.00	11.77
10448	CG1	VAL	C	136	-45.745	-28.715	3.876	1.00	12.54
10452	CG2	VAL	C	136	-43.451	-28.962	4.850	1.00	13.22
10456	C	VAL	C	136	-44.931	-26.433	2.336	1.00	11.72
10457	O	VAL	C	136	-45.488	-26.816	1.308	1.00	11.73
10458	N	ARG	C	137	-45.188	-25.261	2.903	1.00	11.52
10460	CA	ARG	C	137	-46.192	-24.363	2.355	1.00	11.78
10462	CB	ARG	C	137	-46.445	-23.178	3.284	1.00	12.53
10465	CG	ARG	C	137	-47.480	-22.226	2.726	1.00	16.74
10468	CD	ARG	C	137	-47.687	-20.990	3.554	1.00	22.35
10471	NE	ARG	C	137	-48.901	-21.068	4.356	1.00	27.23
10473	CZ	ARG	C	137	-48.987	-21.570	5.577	1.00	29.79
10474	NH1	ARG	C	137	-47.922	-22.078	6.189	1.00	31.32
10477	NH2	ARG	C	137	-50.164	-21.572	6.198	1.00	31.88
10480	C	ARG	C	137	-45.785	-23.855	0.980	1.00	11.68
10481	O	ARG	C	137	-46.595	-23.839	0.058	1.00	10.65
10482	N	LYS	C	138	-44.521	-23.470	0.838	1.00	11.55
10484	CA	LYS	C	138	-44.048	-22.911	-0.428	1.00	12.05
10486	CB	LYS	C	138	-42.644	-22.303	-0.283	1.00	12.70
10489	CG	LYS	C	138	-42.201	-21.476	-1.495	1.00	15.14
10492	CD	LYS	C	138	-40.767	-21.047	-1.340	1.00	19.51
10495	CE	LYS	C	138	-40.347	-20.072	-2.422	1.00	21.97
10498	NZ	LYS	C	138	-39.683	-18.881	-1.838	1.00	23.87
10502	C	LYS	C	138	-44.083	-23.972	-1.516	1.00	11.56
10503	O	LYS	C	138	-44.482	-23.694	-2.644	1.00	11.32
10504	N	SER	C	139	-43.689	-25.201	-1.174	1.00	11.25
10506	CA	SER	C	139	-43.748	-26.306	-2.119	1.00	10.87
10508	CB	SER	C	139	-43.153	-27.573	-1.502	1.00	10.63
10511	OG	SER	C	139	-41.777	-27.404	-1.226	1.00	13.04
10513	C	SER	C	139	-45.194	-26.570	-2.552	1.00	11.08
10514	O	SER	C	139	-45.474	-26.757	-3.732	1.00	11.24
10515	N	MET	C	140	-46.119	-26.553	-1.603	1.00	11.24
10517	CA	MET	C	140	-47.527	-26.766	-1.943	1.00	11.89
10519	CB	MET	C	140	-48.388	-26.910	-0.696	1.00	12.74
10522	CG	MET	C	140	-49.713	-27.599	-0.967	1.00	16.16
10525	SD	MET	C	140	-49.542	-29.206	-1.819	1.00	21.15
10526	CE	MET	C	140	-48.255	-29.937	-0.846	1.00	9.85
10530	C	MET	C	140	-48.059	-25.636	-2.823	1.00	11.41
10531	O	MET	C	140	-48.823	-25.889	-3.744	1.00	11.04
10532	N	GLU	C	141	-47.638	-24.395	-2.574	1.00	10.66
10534	CA	GLU	C	141	-48.147	-23.255	-3.340	1.00	11.39

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
10536	CB	GLU	C	141	-47.757	-21.937	-2.671	1.00	12.34
10539	CG	GLU	C	141	-48.496	-21.654	-1.374	1.00	16.25
10542	CD	GLU	C	141	-49.861	-21.009	-1.558	1.00	21.15
10543	OE1	GLU	C	141	-50.738	-21.270	-0.709	1.00	26.97
10544	OE2	GLU	C	141	-50.062	-20.225	-2.517	1.00	25.27
10545	C	GLU	C	141	-47.594	-23.279	-4.758	1.00	10.61
10546	O	GLU	C	141	-48.354	-23.180	-5.717	1.00	10.81
10547	N	VAL	C	142	-46.279	-23.421	-4.892	1.00	10.06
10549	CA	VAL	C	142	-45.641	-23.324	-6.204	1.00	9.90
10551	CB	VAL	C	142	-44.118	-23.008	-6.097	1.00	9.92
10553	CG1	VAL	C	142	-43.453	-23.014	-7.468	1.00	9.87
10557	CG2	VAL	C	142	-43.890	-21.669	-5.407	1.00	10.73
10561	C	VAL	C	142	-45.848	-24.600	-7.017	1.00	10.12
10562	O	VAL	C	142	-46.123	-24.544	-8.217	1.00	10.04
10563	N	ASN	C	143	-45.646	-25.753	-6.381	1.00	9.30
10565	CA	ASN	C	143	-45.619	-27.016	-7.110	1.00	9.26
10567	CB	ASN	C	143	-44.850	-28.094	-6.344	1.00	8.54
10570	CG	ASN	C	143	-43.393	-27.748	-6.073	1.00	9.98
10571	OD1	ASN	C	143	-42.867	-26.710	-6.491	1.00	9.50
10572	ND2	ASN	C	143	-42.739	-28.626	-5.308	1.00	11.56
10575	C	ASN	C	143	-47.005	-27.593	-7.379	1.00	9.79
10576	O	ASN	C	143	-47.178	-28.405	-8.299	1.00	10.10
10577	N	PHE	C	144	-47.986	-27.199	-6.565	1.00	9.50
10579	CA	PHE	C	144	-49.329	-27.747	-6.659	1.00	9.25
10581	CB	PHE	C	144	-49.690	-28.577	-5.418	1.00	9.31
10584	CG	PHE	C	144	-51.143	-28.925	-5.364	1.00	9.66
10585	CD1	PHE	C	144	-51.662	-29.838	-6.262	1.00	10.31
10587	CE1	PHE	C	144	-53.005	-30.128	-6.279	1.00	11.30
10589	CZ	PHE	C	144	-53.853	-29.510	-5.370	1.00	11.77
10591	CE2	PHE	C	144	-53.340	-28.600	-4.470	1.00	10.72
10593	CD2	PHE	C	144	-52.001	-28.298	-4.474	1.00	11.84
10595	C	PHE	C	144	-50.390	-26.670	-6.917	1.00	9.51
10596	O	PHE	C	144	-51.059	-26.705	-7.939	1.00	9.70
10597	N	LEU	C	145	-50.562	-25.717	-6.005	1.00	9.54
10599	CA	LEU	C	145	-51.674	-24.781	-6.138	1.00	10.24
10601	CB	LEU	C	145	-51.764	-23.827	-4.941	1.00	11.13
10604	CG	LEU	C	145	-53.035	-22.978	-4.915	1.00	15.42
10606	CD1	LEU	C	145	-54.281	-23.835	-4.900	1.00	18.11
10610	CD2	LEU	C	145	-52.986	-22.049	-3.725	1.00	17.85
10614	C	LEU	C	145	-51.573	-23.969	-7.422	1.00	9.65
10615	O	LEU	C	145	-52.574	-23.745	-8.095	1.00	9.94
10616	N	SER	C	146	-50.372	-23.518	-7.761	1.00	9.33
10618	CA	SER	C	146	-50.209	-22.741	-8.995	1.00	9.53
10620	CB	SER	C	146	-48.800	-22.177	-9.133	1.00	9.57
10623	OG	SER	C	146	-47.884	-23.177	-9.512	1.00	9.52
10625	C	SER	C	146	-50.604	-23.538	-10.240	1.00	9.49
10626	O	SER	C	146	-51.140	-22.967	-11.183	1.00	9.66
10627	N	TYR	C	147	-50.385	-24.856	-10.231	1.00	9.39
10629	CA	TYR	C	147	-50.812	-25.701	-11.343	1.00	9.19

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
10631	CB	TYR	C	147	-50.334	-27.151	-11.181	1.00	9.12
10634	CG	TYR	C	147	-48.881	-27.436	-11.480	1.00	9.26
10635	CD1	TYR	C	147	-47.867	-26.518	-11.196	1.00	10.97
10637	CE1	TYR	C	147	-46.535	-26.818	-11.464	1.00	10.28
10639	CZ	TYR	C	147	-46.206	-28.051	-12.024	1.00	9.77
10640	OH	TYR	C	147	-44.890	-28.382	-12.294	1.00	10.98
10642	CE2	TYR	C	147	-47.199	-28.962	-12.304	1.00	10.13
10644	CD2	TYR	C	147	-48.514	-28.655	-12.035	1.00	9.75
10646	C	TYR	C	147	-52.340	-25.695	-11.472	1.00	9.26
10647	O	TYR	C	147	-52.872	-25.682	-12.578	1.00	9.37
10648	N	VAL	C	148	-53.043	-25.727	-10.342	1.00	9.23
10650	CA	VAL	C	148	-54.501	-25.675	-10.351	1.00	9.66
10652	CB	VAL	C	148	-55.083	-26.009	-8.948	1.00	9.79
10654	CG1	VAL	C	148	-54.640	-27.391	-8.499	1.00	10.65
10658	CG2	VAL	C	148	-56.609	-25.937	-8.973	1.00	10.40
10662	C	VAL	C	148	-54.994	-24.314	-10.861	1.00	9.64
10663	O	VAL	C	148	-55.930	-24.243	-11.658	1.00	10.08
10664	N	VAL	C	149	-54.359	-23.238	-10.411	1.00	9.45
10666	CA	VAL	C	149	-54.740	-21.891	-10.817	1.00	9.55
10668	CB	VAL	C	149	-53.965	-20.833	-10.011	1.00	9.47
10670	CG1	VAL	C	149	-54.120	-19.443	-10.612	1.00	10.83
10674	CG2	VAL	C	149	-54.420	-20.861	-8.543	1.00	9.60
10678	C	VAL	C	149	-54.521	-21.709	-12.327	1.00	9.64
10679	O	VAL	C	149	-55.368	-21.146	-13.029	1.00	9.66
10680	N	LEU	C	150	-53.396	-22.200	-12.816	1.00	9.80
10682	CA	LEU	C	150	-53.084	-22.129	-14.242	1.00	9.82
10684	CB	LEU	C	150	-51.663	-22.647	-14.506	1.00	10.08
10687	CG	LEU	C	150	-50.550	-21.736	-13.979	1.00	10.13
10689	CD1	LEU	C	150	-49.245	-22.515	-13.836	1.00	11.23
10693	CD2	LEU	C	150	-50.352	-20.536	-14.870	1.00	9.96
10697	C	LEU	C	150	-54.116	-22.918	-15.059	1.00	10.66
10698	O	LEU	C	150	-54.557	-22.481	-16.124	1.00	10.53
10699	N	THR	C	151	-54.486	-24.090	-14.566	1.00	10.13
10701	CA	THR	C	151	-55.443	-24.950	-15.243	1.00	10.89
10703	CB	THR	C	151	-55.556	-26.292	-14.497	1.00	11.27
10705	OG1	THR	C	151	-54.338	-27.031	-14.658	1.00	11.70
10707	CG2	THR	C	151	-56.627	-27.186	-15.106	1.00	12.94
10711	C	THR	C	151	-56.801	-24.278	-15.328	1.00	10.70
10712	O	THR	C	151	-57.430	-24.265	-16.384	1.00	10.80
10713	N	VAL	C	152	-57.265	-23.720	-14.211	1.00	10.58
10715	CA	VAL	C	152	-58.558	-23.039	-14.192	1.00	11.10
10717	CB	VAL	C	152	-58.908	-22.559	-12.775	1.00	11.01
10719	CG1	VAL	C	152	-60.053	-21.560	-12.796	1.00	11.13
10723	CG2	VAL	C	152	-59.258	-23.745	-11.888	1.00	12.30
10727	C	VAL	C	152	-58.563	-21.883	-15.198	1.00	11.12
10728	O	VAL	C	152	-59.536	-21.705	-15.945	1.00	11.53
10729	N	ALA	C	153	-57.471	-21.123	-15.243	1.00	11.17
10731	CA	ALA	C	153	-57.356	-20.001	-16.169	1.00	11.11
10733	CB	ALA	C	153	-56.117	-19.195	-15.857	1.00	11.65

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
10737	C	ALA	C	153	-57.312	-20.454	-17.639	1.00	11.26
10738	O	ALA	C	153	-57.774	-19.741	-18.521	1.00	11.86
10739	N	ALA	C	154	-56.748	-21.631	-17.882	1.00	10.68
10741	CA	ALA	C	154	-56.537	-22.143	-19.234	1.00	10.86
10743	CB	ALA	C	154	-55.318	-23.041	-19.246	1.00	11.09
10747	C	ALA	C	154	-57.724	-22.920	-19.774	1.00	11.00
10748	O	ALA	C	154	-57.841	-23.112	-20.979	1.00	10.98
10749	N	LEU	C	155	-58.593	-23.393	-18.888	1.00	11.32
10751	CA	LEU	C	155	-59.573	-24.386	-19.301	1.00	12.69
10753	CB	LEU	C	155	-60.326	-24.975	-18.095	1.00	13.05
10756	CG	LEU	C	155	-61.032	-26.308	-18.380	1.00	16.34
10758	CD1	LEU	C	155	-61.870	-26.680	-17.184	1.00	17.18
10762	CD2	LEU	C	155	-60.049	-27.426	-18.721	1.00	16.43
10766	C	LEU	C	155	-60.537	-23.890	-20.389	1.00	12.29
10767	O	LEU	C	155	-60.828	-24.645	-21.303	1.00	12.59
10768	N	PRO	C	156	-61.040	-22.660	-20.325	1.00	12.60
10769	CA	PRO	C	156	-61.903	-22.175	-21.413	1.00	12.23
10771	CB	PRO	C	156	-62.179	-20.722	-21.029	1.00	12.07
10774	CG	PRO	C	156	-62.097	-20.743	-19.525	1.00	12.49
10777	CD	PRO	C	156	-60.948	-21.681	-19.233	1.00	12.50
10780	C	PRO	C	156	-61.263	-22.301	-22.799	1.00	12.23
10781	O	PRO	C	156	-61.921	-22.804	-23.708	1.00	12.31
10782	N	MET	C	157	-60.007	-21.886	-22.934	1.00	11.80
10784	CA	MET	C	157	-59.287	-22.017	-24.202	1.00	11.75
10786	CB	MET	C	157	-57.948	-21.281	-24.164	1.00	11.83
10789	CG	MET	C	157	-58.075	-19.782	-24.274	1.00	12.01
10792	SD	MET	C	157	-56.503	-18.933	-24.344	1.00	13.15
10793	CE	MET	C	157	-55.976	-19.071	-22.645	1.00	14.30
10797	C	MET	C	157	-59.064	-23.478	-24.575	1.00	11.63
10798	O	MET	C	157	-59.162	-23.835	-25.737	1.00	11.83
10799	N	LEU	C	158	-58.726	-24.319	-23.600	1.00	11.15
10801	CA	LEU	C	158	-58.465	-25.732	-23.884	1.00	11.34
10803	CB	LEU	C	158	-57.804	-26.427	-22.691	1.00	11.54
10806	CG	LEU	C	158	-56.426	-25.914	-22.286	1.00	11.46
10808	CD1	LEU	C	158	-56.052	-26.464	-20.916	1.00	12.53
10812	CD2	LEU	C	158	-55.394	-26.290	-23.352	1.00	10.93
10816	C	LEU	C	158	-59.757	-26.455	-24.290	1.00	11.70
10817	O	LEU	C	158	-59.732	-27.348	-25.126	1.00	11.73
10818	N	LYS	C	159	-60.884	-26.039	-23.726	1.00	12.44
10820	CA	LYS	C	159	-62.170	-26.614	-24.114	1.00	13.17
10822	CB	LYS	C	159	-63.279	-26.159	-23.171	1.00	13.26
10825	CG	LYS	C	159	-63.266	-26.899	-21.843	1.00	14.05
10828	CD	LYS	C	159	-64.204	-26.251	-20.837	1.00	15.54
10831	CE	LYS	C	159	-64.426	-27.133	-19.607	1.00	17.54
10834	NZ	LYS	C	159	-65.087	-26.391	-18.494	1.00	19.85
10838	C	LYS	C	159	-62.481	-26.240	-25.560	1.00	13.82
10839	O	LYS	C	159	-62.982	-27.073	-26.324	1.00	13.83
10840	N	GLN	C	160	-62.138	-25.009	-25.946	1.00	14.43
10842	CA	GLN	C	160	-62.353	-24.547	-27.319	1.00	15.11



# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
10844	CB	GLN	C	160	-61.981	-23.060	-27.458	1.00	15.75
10847	CG	GLN	C	160	-62.338	-22.422	-28.784	1.00	19.69
10850	CD	GLN	C	160	-63.744	-21.857	-28.793	1.00	24.32
10851	OE1	GLN	C	160	-63.931	-20.637	-28.716	1.00	29.90
10852	NE2	GLN	C	160	-64.732	-22.733	-28.861	1.00	26.30
10855	C	GLN	C	160	-61.560	-25.373	-28.331	1.00	14.82
10856	O	GLN	C	160	-62.043	-25.660	-29.429	1.00	15.00
10857	N	SER	C	161	-60.348	-25.768	-27.958	1.00	13.58
10859	CA	SER	C	161	-59.432	-26.442	-28.871	1.00	13.34
10861	CB	SER	C	161	-58.009	-25.905	-28.663	1.00	13.59
10864	OG	SER	C	161	-57.547	-26.233	-27.369	1.00	14.26
10866	C	SER	C	161	-59.405	-27.955	-28.701	1.00	13.20
10867	O	SER	C	161	-58.660	-28.636	-29.404	1.00	12.81
10868	N	ASN	C	162	-60.197	-28.488	-27.770	1.00	13.25
10870	CA	ASN	C	162	-60.086	-29.892	-27.384	1.00	13.42
10872	CB	ASN	C	162	-60.640	-30.815	-28.477	1.00	14.20
10875	CG	ASN	C	162	-62.074	-30.484	-28.852	1.00	16.23
10876	OD1	ASN	C	162	-62.950	-30.438	-28.002	1.00	19.16
10877	ND2	ASN	C	162	-62.307	-30.220	-30.135	1.00	22.21
10880	C	ASN	C	162	-58.636	-30.244	-27.061	1.00	12.44
10881	O	ASN	C	162	-58.084	-31.227	-27.562	1.00	11.76
10882	N	GLY	C	163	-58.034	-29.409	-26.216	1.00	11.67
10884	CA	GLY	C	163	-56.622	-29.446	-25.933	1.00	11.43
10887	C	GLY	C	163	-56.204	-30.406	-24.842	1.00	11.08
10888	O	GLY	C	163	-56.880	-31.401	-24.557	1.00	10.37
10889	N	SER	C	164	-55.060	-30.098	-24.245	1.00	10.76
10891	CA	SER	C	164	-54.332	-31.044	-23.410	1.00	11.11
10893	CB	BSER	C	164	-53.332	-31.820	-24.283	0.35	11.22
10894	CB	ASER	C	164	-53.337	-31.830	-24.247	0.65	10.93
10899	OG	BSER	C	164	-52.125	-32.162	-23.610	0.35	12.99
10900	OG	ASER	C	164	-53.977	-32.490	-25.332	0.65	10.55
10903	C	SER	C	164	-53.604	-30.317	-22.286	1.00	11.07
10904	O	SER	C	164	-53.043	-29.222	-22.477	1.00	11.12
10905	N	ILE	C	165	-53.614	-30.940	-21.116	1.00	11.02
10907	CA	ILE	C	165	-52.832	-30.510	-19.971	1.00	10.80
10909	CB	ILE	C	165	-53.726	-30.350	-18.743	1.00	11.30
10911	CG1	ILE	C	165	-54.849	-29.336	-19.019	1.00	11.60
10914	CD1	ILE	C	165	-55.933	-29.326	-17.987	1.00	13.37
10918	CG2	ILE	C	165	-52.896	-29.949	-17.519	1.00	12.80
10922	C	ILE	C	165	-51.781	-31.576	-19.697	1.00	11.02
10923	O	ILE	C	165	-52.106	-32.749	-19.615	1.00	11.76
10924	N	VAL	C	166	-50.526	-31.156	-19.569	1.00	9.66
10926	CA	VAL	C	166	-49.421	-32.043	-19.251	1.00	10.51
10928	CB	VAL	C	166	-48.359	-31.984	-20.369	1.00	10.67
10930	CG1	VAL	C	166	-47.215	-32.939	-20.077	1.00	11.96
10934	CG2	VAL	C	166	-49.003	-32.321	-21.698	1.00	12.13
10938	C	VAL	C	166	-48.854	-31.608	-17.901	1.00	10.66
10939	O	VAL	C	166	-48.458	-30.451	-17.724	1.00	10.78
10940	N	VAL	C	167	-48.838	-32.530	-16.947	1.00	10.45

## FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
10942	CA	VAL	C	167	-48.376	-32.259	-15.601	1.00	10.11
10944	CB	VAL	C	167	-49.436	-32.668	-14.570	1.00	10.54
10946	CG1	VAL	C	167	-48.916	-32.462	-13.150	1.00	11.06
10950	CG2	VAL	C	167	-50.727	-31.894	-14.819	1.00	10.24
10954	C	VAL	C	167	-47.107	-33.059	-15.364	1.00	9.95
10955	O	VAL	C	167	-47.121	-34.284	-15.419	1.00	11.18
10956	N	VAL	C	168	-46.011	-32.375	-15.087	1.00	9.74
10958	CA	VAL	C	168	-44.733	-33.055	-14.887	1.00	9.53
10960	CB	VAL	C	168	-43.544	-32.234	-15.412	1.00	9.85
10962	CG1	VAL	C	168	-42.247	-33.007	-15.232	1.00	10.20
10966	CG2	VAL	C	168	-43.741	-31.871	-16.878	1.00	9.78
10970	C	VAL	C	168	-44.576	-33.420	-13.408	1.00	10.22
10971	O	VAL	C	168	-44.708	-32.589	-12.520	1.00	10.39
10972	N	SER	C	169	-44.336	-34.700	-13.166	1.00	10.11
10974	CA	SER	C	169	-44.179	-35.238	-11.824	1.00	10.92
10976	CB	SER	C	169	-45.449	-35.944	-11.387	1.00	11.42
10979	OG	SER	C	169	-45.409	-36.251	-10.001	1.00	11.77
10981	C	SER	C	169	-42.967	-36.159	-11.789	1.00	10.65
10982	O	SER	C	169	-42.052	-36.010	-12.586	1.00	11.33
10983	N	SER	C	170	-42.969	-37.134	-10.897	1.00	10.80
10985	CA	SER	C	170	-41.735	-37.637	-10.322	1.00	10.54
10987	CB	SER	C	170	-41.365	-36.729	-9.155	1.00	11.04
10990	OG	SER	C	170	-41.518	-35.369	-9.508	1.00	11.64
10992	C	SER	C	170	-41.909	-39.018	-9.746	1.00	10.49
10993	O	SER	C	170	-42.999	-39.369	-9.313	1.00	10.35
10994	N	LEU	C	171	-40.828	-39.790	-9.684	1.00	9.63
10996	CA	LEU	C	171	-40.871	-41.033	-8.913	1.00	9.86
10998	CB	LEU	C	171	-39.511	-41.726	-8.867	1.00	9.95
11001	CG	LEU	C	171	-39.010	-42.313	-10.185	1.00	10.79
11003	CD1	LEU	C	171	-39.924	-43.383	-10.703	1.00	12.00
11007	CD2	LEU	C	171	-37.609	-42.864	-10.006	1.00	10.79
11011	C	LEU	C	171	-41.354	-40.765	-7.480	1.00	9.64
11012	O	LEU	C	171	-42.133	-41.540	-6.936	1.00	10.13
11013	N	ALA	C	172	-40.892	-39.665	-6.885	1.00	9.61
11015	CA	ALA	C	172	-41.286	-39.285	-5.521	1.00	9.96
11017	CB	ALA	C	172	-40.298	-38.278	-4.956	1.00	10.57
11021	C	ALA	C	172	-42.732	-38.740	-5.445	1.00	9.81
11022	O	ALA	C	172	-43.203	-38.331	-4.372	1.00	10.31
11023	N	GLY	C	173	-43.429	-38.746	-6.580	1.00	10.12
11025	CA	GLY	C	173	-44.848	-38.454	-6.648	1.00	10.07
11028	C	GLY	C	173	-45.703	-39.704	-6.792	1.00	10.08
11029	O	GLY	C	173	-46.924	-39.602	-6.924	1.00	10.02
11030	N	LYS	C	174	-45.055	-40.872	-6.767	1.00	10.13
11032	CA	LYS	C	174	-45.723	-42.179	-6.880	1.00	10.29
11034	CB	LYS	C	174	-45.403	-42.838	-8.227	1.00	10.55
11037	CG	LYS	C	174	-46.083	-42.184	-9.412	1.00	10.70
11040	CD	LYS	C	174	-47.591	-42.356	-9.381	1.00	9.89
11043	CE	LYS	C	174	-48.213	-41.984	-10.704	1.00	10.64
11046	NZ	LYS	C	174	-49.689	-42.236	-10.689	1.00	10.05

## FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
11050	C	LYS	C	174	-45.353	-43.143	-5.747	1.00	10.58
11051	O	LYS	C	174	-46.158	-44.004	-5.371	1.00	11.41
11052	N	VAL	C	175	-44.130	-43.025	-5.246	1.00	11.20
11054	CA	VAL	C	175	-43.653	-43.780	-4.103	1.00	11.43
11056	CB	VAL	C	175	-42.750	-44.980	-4.507	1.00	11.37
11058	CG1	VAL	C	175	-41.413	-44.531	-5.080	1.00	12.55
11062	CG2	VAL	C	175	-43.483	-45.898	-5.481	1.00	11.65
11066	C	VAL	C	175	-42.903	-42.838	-3.163	1.00	11.93
11067	O	VAL	C	175	-42.562	-41.716	-3.534	1.00	11.71
11068	N	ALA	C	176	-42.671	-43.302	-1.944	1.00	11.71
11070	CA	ALA	C	176	-42.078	-42.471	-0.901	1.00	12.00
11072	CB	ALA	C	176	-42.707	-42.808	0.454	1.00	12.06
11076	C	ALA	C	176	-40.560	-42.589	-0.815	1.00	12.14
11077	O	ALA	C	176	-39.989	-43.687	-0.876	1.00	13.06
11078	N	TYR	C	177	-39.918	-41.437	-0.640	1.00	12.24
11080	CA	TYR	C	177	-38.492	-41.336	-0.418	1.00	11.81
11082	CB	TYR	C	177	-37.805	-40.651	-1.599	1.00	12.39
11085	CG	TYR	C	177	-37.756	-41.426	-2.873	1.00	11.35
11086	CD1	TYR	C	177	-38.829	-41.431	-3.738	1.00	11.90
11088	CE1	TYR	C	177	-38.787	-42.114	-4.924	1.00	11.56
11090	CZ	TYR	C	177	-37.645	-42.808	-5.264	1.00	11.78
11091	OH	TYR	C	177	-37.602	-43.470	-6.450	1.00	13.49
11093	CE2	TYR	C	177	-36.551	-42.812	-4.437	1.00	11.67
11095	CD2	TYR	C	177	-36.609	-42.117	-3.239	1.00	11.55
11097	C	TYR	C	177	-38.223	-40.450	0.779	1.00	11.91
11098	O	TYR	C	177	-38.912	-39.451	0.955	1.00	12.34
11099	N	PRO	C	178	-37.164	-40.726	1.531	1.00	12.35
11100	CA	PRO	C	178	-36.708	-39.769	2.536	1.00	12.78
11102	CB	PRO	C	178	-35.653	-40.558	3.326	1.00	12.91
11105	CG	PRO	C	178	-35.109	-41.519	2.351	1.00	13.31
11108	CD	PRO	C	178	-36.267	-41.896	1.448	1.00	12.22
11111	C	PRO	C	178	-36.069	-38.581	1.831	1.00	12.83
11112	O	PRO	C	178	-35.661	-38.707	0.681	1.00	12.97
11113	N	MET	C	179	-35.982	-37.459	2.535	1.00	12.85
11115	CA	MET	C	179	-35.233	-36.265	2.122	1.00	13.13
11117	CB	MET	C	179	-33.834	-36.608	1.569	1.00	13.65
11120	CG	MET	C	179	-33.048	-37.602	2.398	1.00	16.60
11123	SD	MET	C	179	-32.943	-37.180	4.133	1.00	23.62
11124	CE	MET	C	179	-31.984	-38.595	4.760	1.00	24.08
11128	C	MET	C	179	-35.955	-35.344	1.140	1.00	12.42
11129	O	MET	C	179	-35.417	-34.298	0.780	1.00	12.54
11130	N	VAL	C	180	-37.180	-35.706	0.754	1.00	11.55
11132	CA	VAL	C	180	-37.981	-34.904	-0.173	1.00	11.53
11134	CB	VAL	C	180	-37.859	-35.450	-1.621	1.00	11.42
11136	CG1	VAL	C	180	-36.467	-35.217	-2.159	1.00	13.39
11140	CG2	VAL	C	180	-38.215	-36.936	-1.675	1.00	13.07
11144	C	VAL	C	180	-39.449	-34.851	0.284	1.00	11.28
11145	O	VAL	C	180	-40.371	-34.893	-0.522	1.00	11.27
11146	N	ALA	C	181	-39.663	-34.742	1.589	1.00	10.97

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
11148	CA	ALA	C	181	-41.022	-34.858	2.131	1.00	10.45
11150	CB	ALA	C	181	-41.005	-34.829	3.650	1.00	10.76
11154	C	ALA	C	181	-41.990	-33.804	1.583	1.00	9.89
11155	O	ALA	C	181	-43.087	-34.140	1.154	1.00	10.31
11156	N	ALA	C	182	-41.585	-32.545	1.609	1.00	9.08
11158	CA	ALA	C	182	-42.436	-31.454	1.155	1.00	9.39
11160	CB	ALA	C	182	-41.798	-30.126	1.482	1.00	9.89
11164	C	ALA	C	182	-42.714	-31.553	-0.340	1.00	9.11
11165	O	ALA	C	182	-43.837	-31.345	-0.806	1.00	9.95
11166	N	TYR	C	183	-41.680	-31.873	-1.104	1.00	9.19
11168	CA	TYR	C	183	-41.821	-32.048	-2.526	1.00	8.92
11170	CB	TYR	C	183	-40.437	-32.315	-3.093	1.00	8.98
11173	CG	TYR	C	183	-40.351	-32.700	-4.541	1.00	9.20
11174	CD1	TYR	C	183	-40.212	-31.731	-5.529	1.00	8.55
11176	CE1	TYR	C	183	-40.089	-32.084	-6.851	1.00	9.04
11178	CZ	TYR	C	183	-40.080	-33.427	-7.208	1.00	8.86
11179	OH	TYR	C	183	-39.897	-33.800	-8.510	1.00	10.98
11181	CE2	TYR	C	183	-40.213	-34.402	-6.251	1.00	9.82
11183	CD2	TYR	C	183	-40.344	-34.032	-4.917	1.00	9.84
11185	C	TYR	C	183	-42.759	-33.197	-2.844	1.00	8.97
11186	O	TYR	C	183	-43.642	-33.080	-3.682	1.00	8.82
11187	N	SER	C	184	-42.553	-34.320	-2.171	1.00	9.22
11189	CA	SER	C	184	-43.375	-35.498	-2.397	1.00	9.36
11191	CB	BSER	C	184	-42.914	-36.652	-1.517	0.35	9.51
11192	CB	ASER	C	184	-42.869	-36.647	-1.517	0.65	9.80
11197	OG	BSER	C	184	-41.639	-37.084	-1.922	0.35	10.14
11198	OG	ASER	C	184	-43.608	-37.836	-1.728	0.65	12.37
11201	C	SER	C	184	-44.838	-35.189	-2.107	1.00	9.21
11202	O	SER	C	184	-45.715	-35.583	-2.859	1.00	9.01
11203	N	ALA	C	185	-45.100	-34.477	-1.023	1.00	9.21
11205	CA	ALA	C	185	-46.471	-34.071	-0.713	1.00	9.21
11207	CB	ALA	C	185	-46.510	-33.180	0.524	1.00	8.89
11211	C	ALA	C	185	-47.108	-33.353	-1.894	1.00	9.11
11212	O	ALA	C	185	-48.246	-33.626	-2.289	1.00	9.42
11213	N	SER	C	186	-46.358	-32.436	-2.486	1.00	9.15
11215	CA	SER	C	186	-46.883	-31.635	-3.570	1.00	9.23
11217	CB	SER	C	186	-45.992	-30.404	-3.818	1.00	10.04
11220	OG	SER	C	186	-44.786	-30.733	-4.452	1.00	10.67
11222	C	SER	C	186	-47.108	-32.452	-4.835	1.00	8.44
11223	O	SER	C	186	-48.066	-32.220	-5.537	1.00	8.67
11224	N	LYS	C	187	-46.237	-33.425	-5.108	1.00	8.52
11226	CA	LYS	C	187	-46.357	-34.217	-6.320	1.00	8.63
11228	CB	LYS	C	187	-45.015	-34.819	-6.710	1.00	8.62
11231	CG	LYS	C	187	-43.977	-33.790	-7.088	1.00	9.99
11234	CD	LYS	C	187	-44.350	-32.999	-8.329	1.00	10.38
11237	CE	LYS	C	187	-43.120	-32.404	-8.989	1.00	12.16
11240	NZ	LYS	C	187	-43.432	-31.591	-10.202	1.00	10.43
11244	C	LYS	C	187	-47.444	-35.280	-6.183	1.00	8.09
11245	O	LYS	C	187	-48.162	-35.546	-7.137	1.00	8.21

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
11246	N	PHE	C	188	-47.548	-35.896	-5.011	1.00	8.80
11248	CA	PHE	C	188	-48.694	-36.746	-4.711	1.00	8.21
11250	CB	PHE	C	188	-48.608	-37.337	-3.285	1.00	8.23
11253	CG	PHE	C	188	-47.864	-38.658	-3.171	1.00	8.88
11254	CD1	PHE	C	188	-48.544	-39.816	-2.781	1.00	9.22
11256	CE1	PHE	C	188	-47.874	-41.036	-2.665	1.00	9.48
11258	CZ	PHE	C	188	-46.518	-41.100	-2.883	1.00	10.66
11260	CE2	PHE	C	188	-45.822	-39.960	-3.242	1.00	9.38
11262	CD2	PHE	C	188	-46.491	-38.742	-3.383	1.00	8.92
11264	C	PHE	C	188	-50.005	-35.941	-4.886	1.00	8.46
11265	O	PHE	C	188	-50.969	-36.432	-5.470	1.00	7.98
11266	N	ALA	C	189	-50.059	-34.710	-4.378	1.00	8.38
11268	CA	ALA	C	189	-51.255	-33.879	-4.509	1.00	8.54
11270	CB	ALA	C	189	-51.072	-32.538	-3.814	1.00	9.41
11274	C	ALA	C	189	-51.661	-33.680	-5.966	1.00	8.74
11275	O	ALA	C	189	-52.856	-33.699	-6.296	1.00	9.40
11276	N	LEU	C	190	-50.678	-33.473	-6.840	1.00	8.78
11278	CA	LEU	C	190	-50.961	-33.356	-8.261	1.00	8.89
11280	CB	LEU	C	190	-49.687	-33.103	-9.059	1.00	8.62
11283	CG	LEU	C	190	-49.028	-31.740	-8.902	1.00	9.75
11285	CD1	LEU	C	190	-47.653	-31.762	-9.583	1.00	9.93
11289	CD2	LEU	C	190	-49.888	-30.632	-9.466	1.00	9.62
11293	C	LEU	C	190	-51.652	-34.598	-8.804	1.00	8.31
11294	O	LEU	C	190	-52.555	-34.492	-9.604	1.00	8.80
11295	N	ASP	C	191	-51.182	-35.776	-8.400	1.00	8.74
11297	CA	ASP	C	191	-51.750	-37.032	-8.879	1.00	9.15
11299	CB	ASP	C	191	-50.912	-38.202	-8.362	1.00	8.59
11302	CG	ASP	C	191	-51.275	-39.537	-8.978	1.00	10.40
11303	OD1	ASP	C	191	-52.113	-39.608	-9.897	1.00	11.97
11304	OD2	ASP	C	191	-50.719	-40.581	-8.575	1.00	11.31
11305	C	ASP	C	191	-53.185	-37.115	-8.428	1.00	9.63
11306	O	ASP	C	191	-54.089	-37.341	-9.228	1.00	10.09
11307	N	GLY	C	192	-53.420	-36.890	-7.137	1.00	9.36
11309	CA	GLY	C	192	-54.774	-36.925	-6.626	1.00	10.23
11312	C	GLY	C	192	-55.701	-35.959	-7.346	1.00	9.90
11313	O	GLY	C	192	-56.786	-36.335	-7.787	1.00	10.69
11314	N	PHE	C	193	-55.280	-34.705	-7.468	1.00	9.49
11316	CA	PHE	C	193	-56.127	-33.683	-8.055	1.00	9.00
11318	CB	PHE	C	193	-55.520	-32.276	-7.931	1.00	8.70
11321	CG	PHE	C	193	-56.433	-31.212	-8.436	1.00	9.06
11322	CD1	PHE	C	193	-56.265	-30.673	-9.705	1.00	11.25
11324	CE1	PHE	C	193	-57.153	-29.713	-10.190	1.00	11.83
11326	CZ	PHE	C	193	-58.207	-29.296	-9.409	1.00	11.61
11328	CE2	PHE	C	193	-58.403	-29.834	-8.152	1.00	11.48
11330	CD2	PHE	C	193	-57.521	-30.802	-7.670	1.00	11.03
11332	C	PHE	C	193	-56.391	-33.946	-9.524	1.00	8.94
11333	O	PHE	C	193	-57.528	-33.995	-9.962	1.00	9.05
11334	N	PHE	C	194	-55.334	-34.076	-10.304	1.00	9.12
11336	CA	PHE	C	194	-55.485	-34.206	-11.751	1.00	9.24

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
11338	CB	PHE	C	194	-54.164	-33.877	-12.461	1.00	9.39
11341	CG	PHE	C	194	-53.896	-32.403	-12.523	1.00	9.84
11342	CD1	PHE	C	194	-53.071	-31.787	-11.594	1.00	10.52
11344	CE1	PHE	C	194	-52.870	-30.406	-11.631	1.00	10.34
11346	CZ	PHE	C	194	-53.486	-29.649	-12.617	1.00	11.68
11348	CE2	PHE	C	194	-54.317	-30.257	-13.538	1.00	10.85
11350	CD2	PHE	C	194	-54.528	-31.621	-13.477	1.00	10.84
11352	C	PHE	C	194	-56.071	-35.535	-12.190	1.00	9.64
11353	O	PHE	C	194	-56.743	-35.603	-13.223	1.00	9.99
11354	N	SER	C	195	-55.832	-36.592	-11.420	1.00	9.87
11356	CA	SER	C	195	-56.431	-37.886	-11.759	1.00	9.68
11358	CB	SER	C	195	-55.732	-39.037	-11.053	1.00	10.48
11361	OG	SER	C	195	-54.361	-39.094	-11.422	1.00	10.88
11363	C	SER	C	195	-57.932	-37.864	-11.450	1.00	10.15
11364	O	SER	C	195	-58.725	-38.504	-12.135	1.00	9.84
11365	N	SER	C	196	-58.329	-37.115	-10.431	1.00	10.68
11367	CA	SER	C	196	-59.753	-36.937	-10.129	1.00	11.00
11369	CB	BSER	C	196	-59.922	-36.276	-8.763	0.35	11.16
11370	CB	ASER	C	196	-59.951	-36.264	-8.760	0.65	10.98
11375	OG	BSER	C	196	-59.388	-37.109	-7.755	0.35	13.05
11376	OG	ASER	C	196	-61.329	-35.968	-8.526	0.65	10.88
11379	C	SER	C	196	-60.453	-36.129	-11.210	1.00	11.18
11380	O	SER	C	196	-61.511	-36.538	-11.711	1.00	10.91
11381	N	ILE	C	197	-59.882	-34.992	-11.609	1.00	11.70
11383	CA	ILE	C	197	-60.540	-34.212	-12.643	1.00	12.40
11385	CB	BILE	C	197	-59.829	-32.832	-12.820	0.35	12.66
11386	CB	AILE	C	197	-60.082	-32.734	-12.757	0.65	13.05
11389	CG1	BILE	C	197	-60.366	-31.818	-11.808	0.35	14.42
11390	CG1	AILE	C	197	-58.606	-32.605	-13.058	0.65	13.34
11395	CD1	BILE	C	197	-59.681	-31.905	-10.522	0.35	15.75
11396	CD1	AILE	C	197	-58.240	-31.268	-13.672	0.65	14.02
11403	CG2	BILE	C	197	-60.020	-32.284	-14.212	0.35	12.73
11404	CG2	AILE	C	197	-60.484	-31.950	-11.468	0.65	13.92
11411	C	ILE	C	197	-60.532	-34.980	-13.972	1.00	11.80
11412	O	ILE	C	197	-61.447	-34.830	-14.750	1.00	11.83
11413	N	ARG	C	198	-59.539	-35.834	-14.210	1.00	11.75
11415	CA	ARG	C	198	-59.571	-36.668	-15.414	1.00	11.78
11417	CB	ARG	C	198	-58.309	-37.541	-15.544	1.00	11.81
11420	CG	ARG	C	198	-58.173	-38.177	-16.916	1.00	12.68
11423	CD	ARG	C	198	-57.122	-39.245	-17.006	1.00	13.32
11426	NE	ARG	C	198	-55.764	-38.721	-16.913	1.00	13.11
11428	CZ	ARG	C	198	-54.905	-38.954	-15.915	1.00	13.98
11429	NH1	ARG	C	198	-55.263	-39.649	-14.843	1.00	13.66
11432	NH2	ARG	C	198	-53.675	-38.454	-15.963	1.00	14.46
11435	C	ARG	C	198	-60.838	-37.529	-15.420	1.00	12.00
11436	O	ARG	C	198	-61.513	-37.637	-16.441	1.00	12.93
11437	N	LYS	C	199	-61.159	-38.127	-14.280	1.00	11.67
11439	CA	LYS	C	199	-62.376	-38.940	-14.169	1.00	12.09
11441	CB	LYS	C	199	-62.518	-39.591	-12.788	1.00	11.99

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
11444	CG	LYS	C	199	-61.418	-40.532	-12.345	1.00	14.00
11447	CD	LYS	C	199	-61.115	-41.620	-13.316	1.00	14.50
11450	CE	LYS	C	199	-60.216	-42.660	-12.662	1.00	14.92
11453	NZ	LYS	C	199	-59.894	-43.821	-13.526	1.00	14.90
11457	C	LYS	C	199	-63.610	-38.064	-14.423	1.00	12.29
11458	O	LYS	C	199	-64.555	-38.476	-15.103	1.00	12.67
11459	N	GLU	C	200	-63.606	-36.856	-13.873	1.00	12.47
11461	CA	GLU	C	200	-64.723	-35.928	-14.059	1.00	13.12
11463	CB	GLU	C	200	-64.537	-34.670	-13.214	1.00	13.30
11466	CG	GLU	C	200	-64.588	-34.948	-11.724	1.00	14.11
11469	CD	GLU	C	200	-64.475	-33.707	-10.865	1.00	13.83
11470	OE1	GLU	C	200	-64.379	-33.867	-9.635	1.00	15.72
11471	OE2	GLU	C	200	-64.507	-32.575	-11.398	1.00	14.40
11472	C	GLU	C	200	-64.913	-35.541	-15.518	1.00	14.02
11473	O	GLU	C	200	-66.040	-35.456	-15.993	1.00	13.78
11474	N	TYR	C	201	-63.811	-35.291	-16.223	1.00	14.32
11476	CA	TYR	C	201	-63.893	-34.882	-17.623	1.00	15.45
11478	CB	TYR	C	201	-62.545	-34.359	-18.136	1.00	15.63
11481	CG	TYR	C	201	-62.103	-33.025	-17.548	1.00	15.54
11482	CD1	TYR	C	201	-62.899	-32.329	-16.634	1.00	16.11
11484	CE1	TYR	C	201	-62.500	-31.124	-16.102	1.00	17.36
11486	CZ	TYR	C	201	-61.287	-30.587	-16.467	1.00	17.96
11487	OH	TYR	C	201	-60.896	-29.390	-15.910	1.00	21.51
11489	CE2	TYR	C	201	-60.465	-31.252	-17.367	1.00	17.82
11491	CD2	TYR	C	201	-60.881	-32.465	-17.903	1.00	17.27
11493	C	TYR	C	201	-64.398	-36.046	-18.470	1.00	16.52
11494	O	TYR	C	201	-65.107	-35.831	-19.450	1.00	16.68
11495	N	SER	C	202	-64.069	-37.278	-18.082	1.00	17.99
11497	CA	SER	C	202	-64.595	-38.444	-18.795	1.00	19.38
11499	CB	BSER	C	202	-63.963	-39.742	-18.285	0.35	19.36
11500	CB	ASER	C	202	-63.939	-39.730	-18.304	0.65	19.51
11505	OG	BSER	C	202	-64.650	-40.873	-18.798	0.35	19.55
11506	OG	ASER	C	202	-62.588	-39.761	-18.714	0.65	20.60
11509	C	SER	C	202	-66.107	-38.529	-18.675	1.00	20.30
11510	O	SER	C	202	-66.800	-38.684	-19.688	1.00	21.51
11511	N	VAL	C	203	-66.631	-38.410	-17.457	1.00	21.13
11513	CA	VAL	C	203	-68.080	-38.534	-17.247	1.00	21.71
11515	CB	VAL	C	203	-68.447	-38.819	-15.762	1.00	21.98
11517	CG1	VAL	C	203	-67.726	-40.053	-15.260	1.00	23.19
11521	CG2	VAL	C	203	-68.150	-37.632	-14.862	1.00	22.59
11525	C	VAL	C	203	-68.870	-37.324	-17.761	1.00	21.49
11526	O	VAL	C	203	-70.019	-37.462	-18.182	1.00	21.51
11527	N	SER	C	204	-68.260	-36.142	-17.748	1.00	21.18
11529	CA	SER	C	204	-68.932	-34.934	-18.222	1.00	21.40
11531	CB	SER	C	204	-68.566	-33.733	-17.344	1.00	21.60
11534	OG	SER	C	204	-67.215	-33.344	-17.502	1.00	23.00
11536	C	SER	C	204	-68.641	-34.650	-19.704	1.00	21.14
11537	O	SER	C	204	-69.092	-33.642	-20.241	1.00	21.54
11538	N	ARG	C	205	-67.902	-35.550	-20.354	1.00	20.92

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
11540	CA	ARG	C	205	-67.552	-35.430	-21.774	1.00	21.11
11542	CB	ARG	C	205	-68.787	-35.675	-22.649	1.00	21.64
11545	CG	ARG	C	205	-69.402	-37.042	-22.437	1.00	24.83
11548	CD	ARG	C	205	-68.577	-38.204	-22.999	1.00	28.80
11551	NE	ARG	C	205	-68.857	-38.461	-24.415	1.00	32.01
11553	CZ	ARG	C	205	-69.936	-39.087	-24.887	1.00	34.42
11554	NH1	ARG	C	205	-70.073	-39.261	-26.199	1.00	35.76
11557	NH2	ARG	C	205	-70.880	-39.542	-24.064	1.00	35.77
11560	C	ARG	C	205	-66.849	-34.113	-22.133	1.00	20.20
11561	O	ARG	C	205	-67.114	-33.498	-23.176	1.00	20.96
11562	N	VAL	C	206	-65.947	-33.686	-21.250	1.00	18.39
11564	CA	VAL	C	206	-65.039	-32.579	-21.517	1.00	17.38
11566	CB	VAL	C	206	-64.593	-31.899	-20.213	1.00	17.01
11568	CG1	VAL	C	206	-63.527	-30.848	-20.473	1.00	16.97
11572	CG2	VAL	C	206	-65.788	-31.280	-19.488	1.00	17.54
11576	C	VAL	C	206	-63.827	-33.154	-22.256	1.00	16.25
11577	O	VAL	C	206	-63.126	-34.018	-21.733	1.00	15.77
11578	N	ASN	C	207	-63.582	-32.669	-23.469	1.00	15.36
11580	CA	ASN	C	207	-62.583	-33.268	-24.353	1.00	15.03
11582	CB	BASN	C	207	-63.064	-33.243	-25.812	0.35	14.94
11583	CB	AASN	C	207	-63.074	-33.231	-25.802	0.65	15.52
11588	CG	BASN	C	207	-62.217	-34.121	-26.728	0.35	15.15
11589	CG	AASN	C	207	-64.321	-34.061	-26.003	0.65	17.58
11590	OD1BASN	C	207		-61.505	-35.016	-26.272	0.35	15.96
11591	OD1AASN	C	207		-64.289	-35.284	-25.856	0.65	21.70
11592	ND2BASN	C	207		-62.284	-33.853	-28.028	0.35	15.46
11593	ND2AASN	C	207		-65.435	-33.404	-26.327	0.65	21.32
11598	C	ASN	C	207	-61.213	-32.590	-24.213	1.00	13.96
11599	O	ASN	C	207	-60.612	-32.131	-25.187	1.00	14.42
11600	N	VAL	C	208	-60.743	-32.553	-22.971	1.00	12.84
11602	CA	VAL	C	208	-59.425	-32.053	-22.602	1.00	12.45
11604	CB	VAL	C	208	-59.520	-30.840	-21.656	1.00	12.09
11606	CG1	VAL	C	208	-58.139	-30.397	-21.200	1.00	12.54
11610	CG2	VAL	C	208	-60.273	-29.675	-22.338	1.00	12.27
11614	C	VAL	C	208	-58.673	-33.200	-21.929	1.00	11.94
11615	O	VAL	C	208	-59.130	-33.761	-20.907	1.00	12.96
11616	N	SER	C	209	-57.547	-33.581	-22.517	1.00	11.04
11618	CA	SER	C	209	-56.753	-34.678	-21.996	1.00	10.80
11620	CB	SER	C	209	-55.973	-35.349	-23.123	1.00	10.79
11623	OG	SER	C	209	-55.001	-34.475	-23.651	1.00	11.51
11625	C	SER	C	209	-55.834	-34.201	-20.872	1.00	11.00
11626	O	SER	C	209	-55.453	-33.041	-20.820	1.00	10.64
11627	N	ILE	C	210	-55.508	-35.123	-19.966	1.00	10.67
11629	CA	ILE	C	210	-54.622	-34.874	-18.840	1.00	10.64
11631	CB	ILE	C	210	-55.406	-34.842	-17.510	1.00	10.99
11633	CG1	ILE	C	210	-56.335	-33.633	-17.515	1.00	12.38
11636	CD1	ILE	C	210	-57.320	-33.597	-16.371	1.00	14.25
11640	CG2	ILE	C	210	-54.444	-34.779	-16.318	1.00	12.39
11644	C	ILE	C	210	-53.574	-35.970	-18.815	1.00	10.42



# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
11645	O	ILE	C	210	-53.893	-37.147	-18.690	1.00	10.52
11646	N	THR	C	211	-52.318	-35.563	-18.932	1.00	10.85
11648	CA	THR	C	211	-51.185	-36.470	-18.954	1.00	10.87
11650	CB	THR	C	211	-50.371	-36.267	-20.245	1.00	11.03
11652	OG1	THR	C	211	-51.191	-36.536	-21.395	1.00	12.04
11654	CG2	THR	C	211	-49.237	-37.257	-20.322	1.00	12.58
11658	C	THR	C	211	-50.301	-36.180	-17.743	1.00	11.25
11659	O	THR	C	211	-49.804	-35.062	-17.600	1.00	11.86
11660	N	LEU	C	212	-50.088	-37.176	-16.891	1.00	10.98
11662	CA	LEU	C	212	-49.179	-37.060	-15.751	1.00	11.24
11664	CB	LEU	C	212	-49.826	-37.696	-14.508	1.00	11.53
11667	CG	LEU	C	212	-49.049	-37.596	-13.190	1.00	12.33
11669	CD1	LEU	C	212	-49.656	-38.530	-12.126	1.00	13.66
11673	CD2	LEU	C	212	-49.026	-36.156	-12.719	1.00	13.88
11677	C	LEU	C	212	-47.870	-37.777	-16.092	1.00	11.11
11678	O	LEU	C	212	-47.883	-38.947	-16.476	1.00	11.80
11679	N	CYS	C	213	-46.745	-37.089	-15.943	1.00	11.36
11681	CA	CYS	C	213	-45.438	-37.642	-16.285	1.00	12.04
11683	CB	CYS	C	213	-44.654	-36.647	-17.128	1.00	12.06
11686	SG	CYS	C	213	-45.567	-36.107	-18.590	1.00	15.58
11687	C	CYS	C	213	-44.674	-37.982	-15.018	1.00	12.03
11688	O	CYS	C	213	-44.601	-37.180	-14.102	1.00	13.42
11689	N	VAL	C	214	-44.099	-39.173	-14.972	1.00	11.13
11691	CA	VAL	C	214	-43.405	-39.682	-13.801	1.00	11.15
11693	CB	VAL	C	214	-44.032	-41.010	-13.341	1.00	11.37
11695	CG1	VAL	C	214	-43.284	-41.597	-12.148	1.00	11.36
11699	CG2	VAL	C	214	-45.500	-40.783	-13.025	1.00	12.19
11703	C	VAL	C	214	-41.941	-39.887	-14.190	1.00	11.10
11704	O	VAL	C	214	-41.614	-40.792	-14.949	1.00	11.55
11705	N	LEU	C	215	-41.072	-39.026	-13.673	1.00	11.10
11707	CA	LEU	C	215	-39.668	-38.979	-14.094	1.00	10.76
11709	CB	LEU	C	215	-39.277	-37.532	-14.413	1.00	11.03
11712	CG	LEU	C	215	-40.113	-36.777	-15.444	1.00	11.45
11714	CD1	LEU	C	215	-39.478	-35.401	-15.705	1.00	11.15
11718	CD2	LEU	C	215	-40.293	-37.563	-16.715	1.00	13.08
11722	C	LEU	C	215	-38.690	-39.502	-13.055	1.00	10.94
11723	O	LEU	C	215	-38.762	-39.144	-11.870	1.00	10.54
11724	N	GLY	C	216	-37.748	-40.318	-13.527	1.00	10.24
11726	CA	GLY	C	216	-36.578	-40.690	-12.761	1.00	10.40
11729	C	GLY	C	216	-35.527	-39.597	-12.799	1.00	10.80
11730	O	GLY	C	216	-35.834	-38.443	-13.054	1.00	10.94
11731	N	LEU	C	217	-34.279	-39.970	-12.549	1.00	10.40
11733	CA	LEU	C	217	-33.170	-39.017	-12.544	1.00	10.31
11735	CB	LEU	C	217	-31.925	-39.654	-11.939	1.00	10.26
11738	CG	LEU	C	217	-30.696	-38.742	-11.917	1.00	11.04
11740	CD1	LEU	C	217	-30.907	-37.484	-11.083	1.00	11.91
11744	CD2	LEU	C	217	-29.505	-39.511	-11.389	1.00	11.15
11748	C	LEU	C	217	-32.864	-38.525	-13.950	1.00	10.26
11749	O	LEU	C	217	-32.544	-39.316	-14.836	1.00	10.40

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
11750	N	ILE	C	218	-32.992	-37.211	-14.139	1.00	10.47
11752	CA	ILE	C	218	-32.748	-36.545	-15.410	1.00	10.15
11754	CB	ILE	C	218	-34.009	-35.772	-15.897	1.00	10.34
11756	CG1	ILE	C	218	-35.283	-36.607	-15.720	1.00	10.79
11759	CD1	ILE	C	218	-35.315	-37.938	-16.450	1.00	12.88
11763	CG2	ILE	C	218	-33.839	-35.343	-17.351	1.00	10.17
11767	C	ILE	C	218	-31.575	-35.587	-15.205	1.00	11.25
11768	O	ILE	C	218	-31.506	-34.911	-14.180	1.00	11.27
11769	N	ASP	C	219	-30.678	-35.516	-16.195	1.00	11.41
11771	CA	ASP	C	219	-29.396	-34.806	-16.065	1.00	12.13
11773	CB	ASP	C	219	-28.362	-35.378	-17.057	1.00	12.25
11776	CG	ASP	C	219	-28.669	-35.039	-18.486	1.00	14.46
11777	OD1	ASP	C	219	-27.884	-35.450	-19.376	1.00	18.63
11778	OD2	ASP	C	219	-29.667	-34.372	-18.819	1.00	15.36
11779	C	ASP	C	219	-29.432	-33.275	-16.155	1.00	12.14
11780	O	ASP	C	219	-28.507	-32.650	-16.689	1.00	13.04
11781	N	THR	C	220	-30.465	-32.653	-15.598	1.00	12.34
11783	CA	THR	C	220	-30.496	-31.202	-15.489	1.00	12.12
11785	CB	THR	C	220	-31.898	-30.714	-15.071	1.00	11.34
11787	OG1	THR	C	220	-32.221	-31.168	-13.736	1.00	10.94
11789	CG2	THR	C	220	-32.983	-31.289	-15.990	1.00	11.15
11793	C	THR	C	220	-29.448	-30.734	-14.487	1.00	12.50
11794	O	THR	C	220	-29.048	-31.487	-13.595	1.00	12.84
11795	N	GLU	C	221	-29.005	-29.491	-14.624	1.00	13.49
11797	CA	GLU	C	221	-28.019	-28.936	-13.696	1.00	14.50
11799	CB	GLU	C	221	-27.656	-27.500	-14.075	1.00	15.68
11802	CG	GLU	C	221	-26.714	-27.401	-15.267	1.00	20.55
11805	CD	GLU	C	221	-25.246	-27.512	-14.885	1.00	25.80
11806	OE1	GLU	C	221	-24.840	-28.565	-14.341	1.00	30.39
11807	OE2	GLU	C	221	-24.488	-26.540	-15.129	1.00	32.37
11808	C	GLU	C	221	-28.523	-29.009	-12.254	1.00	14.20
11809	O	GLU	C	221	-27.784	-29.370	-11.339	1.00	13.80
11810	N	THR	C	222	-29.807	-28.718	-12.070	1.00	13.18
11812	CA	THR	C	222	-30.445	-28.808	-10.762	1.00	12.90
11814	CB	THR	C	222	-31.934	-28.445	-10.879	1.00	12.97
11816	OG1	THR	C	222	-32.050	-27.033	-11.103	1.00	13.26
11818	CG2	THR	C	222	-32.671	-28.687	-9.583	1.00	13.56
11822	C	THR	C	222	-30.278	-30.189	-10.157	1.00	12.67
11823	O	THR	C	222	-29.849	-30.314	-9.023	1.00	13.04
11824	N	ALA	C	223	-30.609	-31.226	-10.919	1.00	12.33
11826	CA	ALA	C	223	-30.535	-32.581	-10.385	1.00	12.40
11828	CB	ALA	C	223	-31.207	-33.562	-11.322	1.00	12.00
11832	C	ALA	C	223	-29.101	-33.017	-10.110	1.00	13.18
11833	O	ALA	C	223	-28.825	-33.611	-9.079	1.00	13.22
11834	N	MET	C	224	-28.193	-32.703	-11.023	1.00	14.67
11836	CA	MET	C	224	-26.810	-33.150	-10.885	1.00	15.66
11838	CB	MET	C	224	-26.025	-32.858	-12.157	1.00	16.02
11841	CG	MET	C	224	-26.544	-33.583	-13.382	1.00	18.03
11844	SD	MET	C	224	-26.776	-35.368	-13.191	1.00	23.43

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
11845	CE	MET	C	224	-28.250	-35.565	-12.482	1.00	24.53
11849	C	MET	C	224	-26.144	-32.521	-9.672	1.00	16.27
11850	O	MET	C	224	-25.335	-33.169	-8.994	1.00	16.17
11851	N	LYS	C	225	-26.500	-31.278	-9.370	1.00	16.66
11853	CA	LYS	C	225	-25.987	-30.626	-8.171	1.00	17.61
11855	CB	LYS	C	225	-26.170	-29.113	-8.281	1.00	18.39
11858	CG	LYS	C	225	-25.185	-28.501	-9.275	1.00	21.20
11861	CD	LYS	C	225	-25.611	-27.144	-9.805	1.00	25.11
11864	CE	LYS	C	225	-24.397	-26.346	-10.296	1.00	26.80
11867	NZ	LYS	C	225	-24.729	-24.945	-10.663	1.00	29.27
11871	C	LYS	C	225	-26.637	-31.202	-6.912	1.00	17.40
11872	O	LYS	C	225	-25.986	-31.403	-5.888	1.00	16.91
11873	N	ALA	C	226	-27.919	-31.524	-7.005	1.00	16.84
11875	CA	ALA	C	226	-28.650	-32.083	-5.876	1.00	17.21
11877	CB	ALA	C	226	-30.130	-32.127	-6.203	1.00	16.94
11881	C	ALA	C	226	-28.177	-33.479	-5.459	1.00	17.65
11882	O	ALA	C	226	-28.246	-33.831	-4.276	1.00	17.84
11883	N	VAL	C	227	-27.701	-34.273	-6.412	1.00	18.15
11885	CA	VAL	C	227	-27.323	-35.658	-6.127	1.00	19.01
11887	CB	VAL	C	227	-27.946	-36.667	-7.137	1.00	18.72
11889	CG1	VAL	C	227	-29.464	-36.517	-7.194	1.00	18.64
11893	CG2	VAL	C	227	-27.323	-36.527	-8.528	1.00	18.71
11897	C	VAL	C	227	-25.807	-35.851	-6.098	1.00	20.43
11898	O	VAL	C	227	-25.323	-36.982	-6.088	1.00	21.02
11899	N	SER	C	228	-25.057	-34.754	-6.085	1.00	21.60
11901	CA	SER	C	228	-23.590	-34.849	-6.109	1.00	23.41
11903	CB	SER	C	228	-22.961	-33.456	-6.189	1.00	23.50
11906	OG	SER	C	228	-23.339	-32.670	-5.075	1.00	25.53
11908	C	SER	C	228	-23.013	-35.619	-4.914	1.00	24.37
11909	O	SER	C	228	-21.969	-36.264	-5.037	1.00	25.17
11910	N	GLY	C	229	-23.681	-35.542	-3.767	1.00	25.54
11912	CA	GLY	C	229	-23.243	-36.235	-2.559	1.00	26.50
11915	C	GLY	C	229	-23.842	-37.616	-2.348	1.00	27.29
11916	O	GLY	C	229	-23.679	-38.202	-1.273	1.00	27.35
11917	N	ILE	C	230	-24.555	-38.120	-3.355	1.00	28.25
11919	CA	ILE	C	230	-25.022	-39.507	-3.390	1.00	29.37
11921	CB	ILE	C	230	-26.544	-39.602	-3.121	1.00	29.53
11923	CG1	ILE	C	230	-27.352	-38.919	-4.231	1.00	30.02
11926	CD1	ILE	C	230	-28.719	-39.552	-4.476	1.00	29.92
11930	CG2	ILE	C	230	-26.885	-38.990	-1.764	1.00	30.30
11934	C	ILE	C	230	-24.669	-40.128	-4.744	1.00	29.62
11935	O	ILE	C	230	-24.208	-41.265	-4.804	1.00	31.08
11936	N	ALA	C	235	-27.850	-40.788	-14.960	1.00	15.59
11938	CA	ALA	C	235	-28.919	-39.824	-15.235	1.00	14.65
11940	CB	ALA	C	235	-28.465	-38.410	-14.887	1.00	14.99
11944	C	ALA	C	235	-29.317	-39.891	-16.701	1.00	14.89
11945	O	ALA	C	235	-28.460	-39.972	-17.583	1.00	15.68
11946	N	ALA	C	236	-30.619	-39.824	-16.965	1.00	14.03
11948	CA	ALA	C	236	-31.125	-39.859	-18.321	1.00	13.49

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
11950	CB	ALA	C	236	-32.552	-40.346	-18.334	1.00	13.29
11954	C	ALA	C	236	-31.012	-38.478	-18.977	1.00	13.32
11955	O	ALA	C	236	-31.017	-37.451	-18.292	1.00	12.80
11956	N	PRO	C	237	-30.886	-38.438	-20.298	1.00	13.16
11957	CA	PRO	C	237	-30.702	-37.160	-20.988	1.00	12.90
11959	CB	PRO	C	237	-30.288	-37.564	-22.406	1.00	13.19
11962	CG	PRO	C	237	-30.549	-39.003	-22.537	1.00	14.25
11965	CD	PRO	C	237	-30.897	-39.586	-21.225	1.00	13.46
11968	C	PRO	C	237	-31.948	-36.281	-21.008	1.00	13.01
11969	O	PRO	C	237	-33.036	-36.746	-21.366	1.00	13.06
11970	N	LYS	C	238	-31.771	-35.018	-20.638	1.00	12.36
11972	CA	LYS	C	238	-32.895	-34.085	-20.538	1.00	12.40
11974	CB	LYS	C	238	-32.469	-32.768	-19.875	1.00	12.37
11977	CG	LYS	C	238	-31.353	-32.003	-20.575	1.00	13.16
11980	CD	LYS	C	238	-30.933	-30.777	-19.797	1.00	14.89
11983	CE	LYS	C	238	-29.845	-30.009	-20.527	1.00	15.48
11986	NZ	LYS	C	238	-29.391	-28.779	-19.809	1.00	18.83
11990	C	LYS	C	238	-33.575	-33.831	-21.882	1.00	12.76
11991	O	LYS	C	238	-34.787	-33.627	-21.922	1.00	12.67
11992	N	GLU	C	239	-32.817	-33.879	-22.985	1.00	13.42
11994	CA	GLU	C	239	-33.411	-33.666	-24.303	1.00	14.33
11996	CB	GLU	C	239	-32.339	-33.580	-25.397	1.00	15.64
11999	CG	GLU	C	239	-32.891	-33.217	-26.772	1.00	20.08
12002	CD	GLU	C	239	-31.823	-33.076	-27.845	1.00	25.16
12003	OE1	GLU	C	239	-32.189	-33.077	-29.045	1.00	28.77
12004	OE2	GLU	C	239	-30.627	-32.960	-27.502	1.00	30.13
12005	C	GLU	C	239	-34.399	-34.778	-24.633	1.00	13.73
12006	O	GLU	C	239	-35.477	-34.517	-25.155	1.00	12.94
12007	N	GLU	C	240	-34.031	-36.020	-24.338	1.00	13.83
12009	CA	GLU	C	240	-34.915	-37.152	-24.640	1.00	13.97
12011	CB	GLU	C	240	-34.173	-38.487	-24.532	1.00	14.80
12014	CG	GLU	C	240	-35.045	-39.698	-24.842	1.00	18.44
12017	CD	GLU	C	240	-34.277	-41.011	-24.846	1.00	23.31
12018	OE1	GLU	C	240	-33.969	-41.547	-23.758	1.00	24.72
12019	OE2	GLU	C	240	-33.986	-41.519	-25.952	1.00	27.48
12020	C	GLU	C	240	-36.124	-37.151	-23.710	1.00	13.03
12021	O	GLU	C	240	-37.238	-37.451	-24.136	1.00	12.63
12022	N	CYS	C	241	-35.890	-36.836	-22.441	1.00	12.26
12024	CA	CYS	C	241	-36.963	-36.737	-21.457	1.00	12.13
12026	CB	CYS	C	241	-36.392	-36.230	-20.132	1.00	12.21
12029	SG	CYS	C	241	-37.622	-36.092	-18.819	1.00	12.92
12030	C	CYS	C	241	-38.032	-35.766	-21.952	1.00	11.54
12031	O	CYS	C	241	-39.220	-36.070	-21.956	1.00	11.42
12032	N	ALA	C	242	-37.588	-34.585	-22.354	1.00	11.14
12034	CA	ALA	C	242	-38.478	-33.533	-22.820	1.00	10.68
12036	CB	ALA	C	242	-37.664	-32.300	-23.182	1.00	11.33
12040	C	ALA	C	242	-39.311	-34.010	-24.011	1.00	11.02
12041	O	ALA	C	242	-40.508	-33.735	-24.095	1.00	10.47
12042	N	LEU	C	243	-38.691	-34.742	-24.935	1.00	11.46

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
12044	CA	LEU	C	243	-39.415	-35.218	-26.098	1.00	12.20
12046	CB	LEU	C	243	-38.459	-35.808	-27.135	1.00	12.99
12049	CG	LEU	C	243	-39.123	-36.281	-28.423	1.00	14.19
12051	CD1	LEU	C	243	-39.909	-35.153	-29.077	1.00	14.92
12055	CD2	LEU	C	243	-38.075	-36.848	-29.373	1.00	15.95
12059	C	LEU	C	243	-40.476	-36.236	-25.698	1.00	12.29
12060	O	LEU	C	243	-41.580	-36.192	-26.204	1.00	12.28
12061	N	GLU	C	244	-40.165	-37.128	-24.763	1.00	12.61
12063	CA	GLU	C	244	-41.139	-38.140	-24.359	1.00	12.79
12065	CB	GLU	C	244	-40.481	-39.215	-23.493	1.00	13.07
12068	CG	GLU	C	244	-39.460	-40.062	-24.238	1.00	15.24
12071	CD	GLU	C	244	-40.019	-40.742	-25.481	1.00	19.30
12072	OE1	GLU	C	244	-39.317	-40.734	-26.519	1.00	21.69
12073	OE2	GLU	C	244	-41.158	-41.257	-25.427	1.00	20.80
12074	C	GLU	C	244	-42.341	-37.532	-23.650	1.00	12.17
12075	O	GLU	C	244	-43.460	-38.036	-23.774	1.00	12.48
12076	N	ILE	C	245	-42.125	-36.448	-22.906	1.00	11.79
12078	CA	ILE	C	245	-43.231	-35.739	-22.267	1.00	11.17
12080	CB	ILE	C	245	-42.710	-34.617	-21.356	1.00	11.19
12082	CG1	ILE	C	245	-41.996	-35.194	-20.122	1.00	10.84
12085	CD1	ILE	C	245	-41.195	-34.156	-19.336	1.00	10.48
12089	CG2	ILE	C	245	-43.867	-33.710	-20.939	1.00	11.40
12093	C	ILE	C	245	-44.164	-35.173	-23.336	1.00	11.48
12094	O	ILE	C	245	-45.370	-35.346	-23.263	1.00	11.59
12095	N	ILE	C	246	-43.598	-34.494	-24.330	1.00	11.41
12097	CA	ILE	C	246	-44.388	-33.923	-25.420	1.00	11.80
12099	CB	ILE	C	246	-43.494	-33.127	-26.399	1.00	11.94
12101	CG1	ILE	C	246	-42.957	-31.862	-25.717	1.00	12.20
12104	CD1	ILE	C	246	-41.738	-31.301	-26.365	1.00	12.71
12108	CG2	ILE	C	246	-44.253	-32.759	-27.670	1.00	12.43
12112	C	ILE	C	246	-45.165	-35.010	-26.159	1.00	12.06
12113	O	ILE	C	246	-46.335	-34.823	-26.478	1.00	12.63
12114	N	LYS	C	247	-44.506	-36.133	-26.431	1.00	12.28
12116	CA	LYS	C	247	-45.114	-37.221	-27.190	1.00	13.13
12118	CB	LYS	C	247	-44.121	-38.368	-27.402	1.00	13.19
12121	CG	LYS	C	247	-42.983	-38.123	-28.371	1.00	16.39
12124	CD	LYS	C	247	-42.235	-39.445	-28.601	1.00	18.33
12127	CE	LYS	C	247	-41.095	-39.338	-29.581	1.00	21.36
12130	NZ	LYS	C	247	-40.239	-40.570	-29.497	1.00	22.66
12134	C	LYS	C	247	-46.319	-37.744	-26.434	1.00	13.16
12135	O	LYS	C	247	-47.371	-37.964	-27.014	1.00	13.27
12136	N	GLY	C	248	-46.164	-37.933	-25.123	1.00	13.15
12138	CA	GLY	C	248	-47.251	-38.404	-24.292	1.00	13.13
12141	C	GLY	C	248	-48.447	-37.484	-24.289	1.00	12.70
12142	O	GLY	C	248	-49.584	-37.937	-24.384	1.00	13.09
12143	N	GLY	C	249	-48.203	-36.184	-24.162	1.00	12.55
12145	CA	GLY	C	249	-49.259	-35.187	-24.204	1.00	12.63
12148	C	GLY	C	249	-49.962	-35.144	-25.545	1.00	12.79
12149	O	GLY	C	249	-51.187	-35.059	-25.606	1.00	13.00

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
12150	N	ALA	C	250	-49.181	-35.206	-26.621	1.00	12.39
12152	CA	ALA	C	250	-49.719	-35.150	-27.982	1.00	12.27
12154	CB	ALA	C	250	-48.601	-35.081	-28.990	1.00	12.75
12158	C	ALA	C	250	-50.605	-36.351	-28.268	1.00	12.07
12159	O	ALA	C	250	-51.627	-36.214	-28.931	1.00	13.44
12160	N	LEU	C	251	-50.210	-37.512	-27.750	1.00	11.77
12162	CA	LEU	C	251	-50.968	-38.757	-27.916	1.00	11.68
12164	CB	LEU	C	251	-50.025	-39.953	-27.845	1.00	11.90
12167	CG	LEU	C	251	-49.059	-40.076	-29.033	1.00	13.00
12169	CD1	LEU	C	251	-48.107	-41.240	-28.818	1.00	14.12
12173	CD2	LEU	C	251	-49.808	-40.207	-30.341	1.00	13.94
12177	C	LEU	C	251	-52.092	-38.910	-26.885	1.00	11.97
12178	O	LEU	C	251	-52.818	-39.909	-26.899	1.00	12.23
12179	N	ARG	C	252	-52.230	-37.926	-26.000	1.00	12.03
12181	CA	ARG	C	252	-53.304	-37.886	-25.000	1.00	12.27
12183	CB	ARG	C	252	-54.678	-37.736	-25.671	1.00	12.40
12186	CG	ARG	C	252	-54.761	-36.562	-26.625	1.00	13.25
12189	CD	ARG	C	252	-56.091	-36.454	-27.343	1.00	12.65
12192	NE	ARG	C	252	-57.130	-35.762	-26.588	1.00	13.17
12194	CZ	ARG	C	252	-57.264	-34.443	-26.497	1.00	12.51
12195	NH1	ARG	C	252	-56.405	-33.625	-27.079	1.00	12.96
12198	NH2	ARG	C	252	-58.272	-33.925	-25.808	1.00	12.62
12201	C	ARG	C	252	-53.264	-39.092	-24.063	1.00	12.06
12202	O	ARG	C	252	-54.299	-39.610	-23.648	1.00	12.00
12203	N	GLN	C	253	-52.056	-39.534	-23.730	1.00	12.30
12205	CA	GLN	C	253	-51.856	-40.656	-22.818	1.00	12.53
12207	CB	GLN	C	253	-50.400	-41.140	-22.885	1.00	13.27
12210	CG	GLN	C	253	-50.010	-41.784	-24.193	1.00	15.78
12213	CD	GLN	C	253	-48.520	-42.133	-24.255	1.00	17.39
12214	OE1	GLN	C	253	-47.810	-42.089	-23.242	1.00	23.39
12215	NE2	GLN	C	253	-48.056	-42.497	-25.433	1.00	23.94
12218	C	GLN	C	253	-52.152	-40.206	-21.390	1.00	12.57
12219	O	GLN	C	253	-51.904	-39.054	-21.039	1.00	12.59
12220	N	GLU	C	254	-52.668	-41.107	-20.561	1.00	12.68
12222	CA	GLU	C	254	-52.905	-40.763	-19.155	1.00	12.99
12224	CB	GLU	C	254	-53.726	-41.842	-18.440	1.00	13.57
12227	CG	GLU	C	254	-55.188	-41.885	-18.868	1.00	16.45
12230	CD	GLU	C	254	-56.106	-42.603	-17.879	1.00	20.30
12231	OE1	GLU	C	254	-57.265	-42.878	-18.247	1.00	26.45
12232	OE2	GLU	C	254	-55.698	-42.886	-16.739	1.00	25.89
12233	C	GLU	C	254	-51.612	-40.511	-18.399	1.00	12.99
12234	O	GLU	C	254	-51.515	-39.548	-17.640	1.00	12.12
12235	N	GLU	C	255	-50.620	-41.373	-18.602	1.00	13.42
12237	CA	GLU	C	255	-49.348	-41.265	-17.891	1.00	14.07
12239	CB	GLU	C	255	-49.344	-42.171	-16.640	1.00	15.08
12242	CG	GLU	C	255	-50.429	-41.781	-15.638	1.00	15.86
12245	CD	GLU	C	255	-50.358	-42.485	-14.288	1.00	19.79
12246	OE1	GLU	C	255	-50.838	-41.887	-13.298	1.00	19.00
12247	OE2	GLU	C	255	-49.865	-43.635	-14.213	1.00	21.69

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
12248	C	GLU	C	255	-48.167	-41.561	-18.811	1.00	14.54
12249	O	GLU	C	255	-48.289	-42.320	-19.783	1.00	15.85
12250	N	VAL	C	256	-47.043	-40.916	-18.518	1.00	13.79
12252	CA	VAL	C	256	-45.763	-41.163	-19.174	1.00	14.05
12254	CB	VAL	C	256	-45.231	-39.901	-19.878	1.00	14.24
12256	CG1	VAL	C	256	-43.779	-40.084	-20.369	1.00	15.45
12260	CG2	VAL	C	256	-46.154	-39.462	-21.009	1.00	15.91
12264	C	VAL	C	256	-44.783	-41.511	-18.073	1.00	13.66
12265	O	VAL	C	256	-44.728	-40.812	-17.072	1.00	13.87
12266	N	TYR	C	257	-44.015	-42.580	-18.263	1.00	12.64
12268	CA	TYR	C	257	-42.942	-42.966	-17.341	1.00	12.61
12270	CB	TYR	C	257	-43.192	-44.374	-16.789	1.00	12.98
12273	CG	TYR	C	257	-44.389	-44.438	-15.867	1.00	13.54
12274	CD1	TYR	C	257	-45.671	-44.561	-16.372	1.00	16.99
12276	CE1	TYR	C	257	-46.778	-44.592	-15.522	1.00	16.68
12278	CZ	TYR	C	257	-46.589	-44.491	-14.162	1.00	16.74
12279	OH	TYR	C	257	-47.684	-44.541	-13.314	1.00	18.08
12281	CE2	TYR	C	257	-45.317	-44.376	-13.641	1.00	16.63
12283	CD2	TYR	C	257	-44.232	-44.338	-14.493	1.00	15.20
12285	C	TYR	C	257	-41.611	-42.898	-18.090	1.00	12.31
12286	O	TYR	C	257	-41.459	-43.476	-19.177	1.00	12.69
12287	N	TYR	C	258	-40.653	-42.164	-17.536	1.00	11.52
12289	CA	TYR	C	258	-39.366	-41.988	-18.194	1.00	11.61
12291	CB	TYR	C	258	-39.301	-40.641	-18.941	1.00	11.76
12294	CG	TYR	C	258	-38.003	-40.489	-19.681	1.00	12.60
12295	CD1	TYR	C	258	-36.944	-39.800	-19.119	1.00	13.41
12297	CE1	TYR	C	258	-35.737	-39.693	-19.774	1.00	14.57
12299	CZ	TYR	C	258	-35.571	-40.271	-21.006	1.00	15.50
12300	OH	TYR	C	258	-34.354	-40.155	-21.640	1.00	18.37
12302	CE2	TYR	C	258	-36.606	-40.971	-21.594	1.00	15.20
12304	CD2	TYR	C	258	-37.822	-41.068	-20.928	1.00	15.06
12306	C	TYR	C	258	-38.233	-42.098	-17.190	1.00	11.75
12307	O	TYR	C	258	-38.245	-41.454	-16.134	1.00	11.72
12308	N	ASP	C	259	-37.264	-42.946	-17.521	1.00	11.55
12310	CA	ASP	C	259	-36.098	-43.218	-16.688	1.00	12.47
12312	CB	ASP	C	259	-36.444	-44.209	-15.578	1.00	12.44
12315	CG	ASP	C	259	-35.344	-44.328	-14.538	1.00	13.61
12316	OD1	ASP	C	259	-34.579	-45.335	-14.508	1.00	13.32
12317	OD2	ASP	C	259	-35.178	-43.439	-13.698	1.00	15.07
12318	C	ASP	C	259	-35.007	-43.834	-17.574	1.00	13.04
12319	O	ASP	C	259	-35.299	-44.365	-18.645	1.00	14.14
12320	N	SER	C	260	-33.770	-43.806	-17.096	1.00	13.75
12322	CA	SER	C	260	-32.660	-44.475	-17.785	1.00	14.36
12324	CB	SER	C	260	-31.336	-44.241	-17.048	1.00	14.73
12327	OG	SER	C	260	-30.898	-42.903	-17.163	1.00	18.81
12329	C	SER	C	260	-32.869	-45.981	-17.908	1.00	14.41
12330	O	SER	C	260	-32.357	-46.597	-18.842	1.00	15.00
12331	N	SER	C	261	-33.603	-46.572	-16.970	1.00	14.01
12333	CA	SER	C	261	-33.740	-48.025	-16.894	1.00	13.87

## FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
12335	CB	SER	C	261	-33.253	-48.514	-15.543	1.00	14.49
12338	OG	SER	C	261	-33.361	-49.932	-15.455	1.00	15.84
12340	C	SER	C	261	-35.180	-48.483	-17.087	1.00	13.53
12341	O	SER	C	261	-36.104	-47.920	-16.487	1.00	12.62
12342	N	LEU	C	262	-35.355	-49.525	-17.896	1.00	13.00
12344	CA	LEU	C	262	-36.642	-50.212	-18.006	1.00	13.34
12346	CB	LEU	C	262	-36.623	-51.231	-19.154	1.00	13.85
12349	CG	LEU	C	262	-36.748	-50.638	-20.563	1.00	15.75
12351	CD1	LEU	C	262	-36.296	-51.629	-21.632	1.00	17.50
12355	CD2	LEU	C	262	-38.183	-50.196	-20.829	1.00	17.92
12359	C	LEU	C	262	-37.055	-50.903	-16.704	1.00	13.03
12360	O	LEU	C	262	-38.243	-51.147	-16.491	1.00	12.35
12361	N	TRP	C	263	-36.106	-51.245	-15.830	1.00	12.74
12363	CA	TRP	C	263	-36.481	-51.756	-14.508	1.00	12.55
12365	CB	TRP	C	263	-35.256	-52.068	-13.646	1.00	12.84
12368	CG	TRP	C	263	-34.510	-53.295	-14.100	1.00	12.36
12369	CD1	TRP	C	263	-33.638	-53.389	-15.139	1.00	13.05
12371	NE1	TRP	C	263	-33.161	-54.671	-15.244	1.00	11.54
12373	CE2	TRP	C	263	-33.727	-55.438	-14.263	1.00	11.98
12374	CD2	TRP	C	263	-34.583	-54.605	-13.523	1.00	12.40
12375	CE3	TRP	C	263	-35.291	-55.160	-12.449	1.00	13.26
12377	CZ3	TRP	C	263	-35.115	-56.506	-12.157	1.00	13.17
12379	CH2	TRP	C	263	-34.256	-57.298	-12.911	1.00	12.56
12381	CZ2	TRP	C	263	-33.559	-56.789	-13.968	1.00	11.95
12383	C	TRP	C	263	-37.374	-50.747	-13.794	1.00	12.35
12384	O	TRP	C	263	-38.355	-51.122	-13.192	1.00	12.64
12385	N	THR	C	264	-37.022	-49.469	-13.894	1.00	11.86
12387	CA	THR	C	264	-37.807	-48.413	-13.274	1.00	11.60
12389	CB	THR	C	264	-37.024	-47.096	-13.293	1.00	11.77
12391	OG1	THR	C	264	-35.732	-47.279	-12.693	1.00	12.80
12393	CG2	THR	C	264	-37.718	-46.041	-12.450	1.00	11.94
12397	C	THR	C	264	-39.139	-48.217	-13.968	1.00	11.37
12398	O	THR	C	264	-40.174	-48.249	-13.319	1.00	11.86
12399	N	THR	C	265	-39.130	-47.998	-15.280	1.00	11.28
12401	CA	THR	C	265	-40.368	-47.602	-15.950	1.00	11.73
12403	CB	THR	C	265	-40.135	-47.039	-17.361	1.00	11.94
12405	OG1	THR	C	265	-39.498	-48.015	-18.182	1.00	12.80
12407	CG2	THR	C	265	-39.170	-45.865	-17.326	1.00	12.88
12411	C	THR	C	265	-41.398	-48.728	-15.994	1.00	12.33
12412	O	THR	C	265	-42.597	-48.461	-15.936	1.00	13.36
12413	N	LEU	C	266	-40.940	-49.973	-16.056	1.00	12.18
12415	CA	LEU	C	266	-41.865	-51.104	-16.103	1.00	12.10
12417	CB	LEU	C	266	-41.212	-52.335	-16.751	1.00	12.70
12420	CG	LEU	C	266	-40.830	-52.222	-18.233	1.00	12.88
12422	CD1	LEU	C	266	-40.131	-53.496	-18.728	1.00	14.06
12426	CD2	LEU	C	266	-42.064	-51.924	-19.085	1.00	15.54
12430	C	LEU	C	266	-42.410	-51.438	-14.711	1.00	12.64
12431	O	LEU	C	266	-43.595	-51.750	-14.570	1.00	13.23
12432	N	LEU	C	267	-41.565	-51.391	-13.684	1.00	12.34



# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
12434	CA	LEU	C	267	-42.001	-51.818	-12.342	1.00	13.06
12436	CB	LEU	C	267	-40.828	-52.378	-11.527	1.00	13.18
12439	CG	LEU	C	267	-40.198	-53.656	-12.083	1.00	14.62
12441	CD1	LEU	C	267	-38.906	-53.953	-11.365	1.00	15.80
12445	CD2	LEU	C	267	-41.172	-54.848	-12.003	1.00	16.24
12449	C	LEU	C	267	-42.744	-50.763	-11.531	1.00	13.48
12450	O	LEU	C	267	-43.542	-51.114	-10.677	1.00	12.93
12451	N	ILE	C	268	-42.480	-49.484	-11.784	1.00	14.13
12453	CA	ILE	C	268	-43.139	-48.401	-11.047	1.00	14.75
12455	CB	ILE	C	268	-42.415	-47.054	-11.288	1.00	14.94
12457	CG1	ILE	C	268	-42.883	-45.980	-10.293	1.00	18.07
12460	CD1	ILE	C	268	-42.227	-46.069	-8.978	1.00	20.18
12464	CG2	ILE	C	268	-42.655	-46.565	-12.688	1.00	16.47
12468	C	ILE	C	268	-44.619	-48.283	-11.421	1.00	14.81
12469	O	ILE	C	268	-45.409	-47.721	-10.666	1.00	14.87
12470	N	ARG	C	269	-44.991	-48.806	-12.588	1.00	14.93
12472	CA	ARG	C	269	-46.384	-48.753	-13.020	1.00	15.70
12474	CB	ARG	C	269	-46.524	-49.279	-14.446	1.00	16.47
12477	CG	ARG	C	269	-46.020	-48.269	-15.468	1.00	19.82
12480	CD	ARG	C	269	-45.925	-48.799	-16.894	1.00	25.74
12483	NE	ARG	C	269	-46.030	-47.721	-17.884	1.00	29.72
12485	CZ	ARG	C	269	-47.152	-47.076	-18.203	1.00	32.58
12486	NH1	ARG	C	269	-47.121	-46.110	-19.118	1.00	34.25
12489	NH2	ARG	C	269	-48.312	-47.381	-17.621	1.00	35.19
12492	C	ARG	C	269	-47.246	-49.564	-12.066	1.00	14.74
12493	O	ARG	C	269	-46.844	-50.628	-11.600	1.00	14.91
12494	N	ASN	C	270	-48.431	-49.035	-11.766	1.00	14.52
12496	CA	ASN	C	270	-49.393	-49.684	-10.882	1.00	13.63
12498	CB	ASN	C	270	-49.614	-48.776	-9.653	1.00	13.49
12501	CG	ASN	C	270	-50.562	-49.361	-8.619	1.00	13.92
12502	OD1	ASN	C	270	-51.013	-48.652	-7.701	1.00	15.25
12503	ND2	ASN	C	270	-50.856	-50.636	-8.744	1.00	12.89
12506	C	ASN	C	270	-50.704	-49.929	-11.655	1.00	13.37
12507	O	ASN	C	270	-51.695	-49.217	-11.448	1.00	12.45
12508	N	PRO	C	271	-50.724	-50.901	-12.572	1.00	13.12
12509	CA	PRO	C	271	-51.937	-51.165	-13.357	1.00	12.95
12511	CB	PRO	C	271	-51.543	-52.340	-14.265	1.00	13.18
12514	CG	PRO	C	271	-50.332	-52.932	-13.650	1.00	13.46
12517	CD	PRO	C	271	-49.628	-51.812	-12.944	1.00	13.41
12520	C	PRO	C	271	-53.136	-51.533	-12.509	1.00	12.78
12521	O	PRO	C	271	-54.260	-51.289	-12.937	1.00	12.71
12522	N	SER	C	272	-52.908	-52.117	-11.341	1.00	12.01
12524	CA	SER	C	272	-54.002	-52.507	-10.460	1.00	11.99
12526	CB	SER	C	272	-53.470	-53.246	-9.231	1.00	12.81
12529	OG	SER	C	272	-52.989	-54.534	-9.597	1.00	14.99
12531	C	SER	C	272	-54.841	-51.319	-10.014	1.00	11.35
12532	O	SER	C	272	-56.058	-51.439	-9.875	1.00	11.41
12533	N	ARG	C	273	-54.207	-50.174	-9.781	1.00	10.61
12535	CA	ARG	C	273	-54.970	-48.965	-9.443	1.00	10.56

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
12537	CB	ARG	C	273	-54.043	-47.774	-9.165	1.00	10.09
12540	CG	ARG	C	273	-54.736	-46.418	-9.209	1.00	9.69
12543	CD	ARG	C	273	-53.908	-45.238	-8.678	1.00	10.35
12546	NE	ARG	C	273	-54.400	-43.988	-9.241	1.00	11.05
12548	CZ	ARG	C	273	-53.748	-42.840	-9.198	1.00	10.78
12549	NH1	ARG	C	273	-52.597	-42.745	-8.556	1.00	11.38
12552	NH2	ARG	C	273	-54.260	-41.784	-9.804	1.00	11.11
12555	C	ARG	C	273	-55.989	-48.612	-10.528	1.00	11.27
12556	O	ARG	C	273	-57.159	-48.355	-10.229	1.00	10.92
12557	N	LYS	C	274	-55.562	-48.609	-11.790	1.00	12.16
12559	CA	LYS	C	274	-56.445	-48.218	-12.890	1.00	13.62
12561	CB	LYS	C	274	-55.659	-48.054	-14.198	1.00	14.83
12564	CG	LYS	C	274	-54.447	-47.103	-14.118	1.00	18.31
12567	CD	LYS	C	274	-54.810	-45.619	-13.969	1.00	22.54
12570	CE	LYS	C	274	-53.569	-44.722	-13.797	1.00	24.36
12573	NZ	LYS	C	274	-53.846	-43.320	-13.308	1.00	25.56
12577	C	LYS	C	274	-57.574	-49.241	-13.058	1.00	13.93
12578	O	LYS	C	274	-58.709	-48.893	-13.372	1.00	13.23
12579	N	ILE	C	275	-57.252	-50.505	-12.833	1.00	15.40
12581	CA	ILE	C	275	-58.246	-51.574	-12.898	1.00	16.26
12583	CB	ILE	C	275	-57.555	-52.942	-12.792	1.00	16.49
12585	CG1	ILE	C	275	-56.826	-53.257	-14.110	1.00	17.58
12588	CD1	ILE	C	275	-55.759	-54.334	-13.987	1.00	19.28
12592	CG2	ILE	C	275	-58.558	-54.044	-12.453	1.00	17.69
12596	C	ILE	C	275	-59.313	-51.385	-11.806	1.00	16.51
12597	O	ILE	C	275	-60.507	-51.477	-12.079	1.00	16.64
12598	N	LEU	C	276	-58.892	-51.123	-10.574	1.00	16.80
12600	CA	LEU	C	276	-59.847	-50.918	-9.481	1.00	17.40
12602	CB	LEU	C	276	-59.154	-50.846	-8.129	1.00	17.71
12605	CG	LEU	C	276	-58.562	-52.175	-7.665	1.00	20.24
12607	CD1	LEU	C	276	-57.740	-51.993	-6.400	1.00	22.08
12611	CD2	LEU	C	276	-59.668	-53.217	-7.446	1.00	20.01
12615	C	LEU	C	276	-60.709	-49.677	-9.717	1.00	17.22
12616	O	LEU	C	276	-61.913	-49.722	-9.529	1.00	17.27
12617	N	GLU	C	277	-60.108	-48.584	-10.175	1.00	16.44
12619	CA	GLU	C	277	-60.890	-47.395	-10.523	1.00	16.53
12621	CB	GLU	C	277	-59.990	-46.275	-11.055	1.00	16.41
12624	CG	GLU	C	277	-59.058	-45.718	-9.993	1.00	15.89
12627	CD	GLU	C	277	-57.953	-44.850	-10.553	1.00	16.14
12628	OE1	GLU	C	277	-57.153	-44.323	-9.747	1.00	16.19
12629	OE2	GLU	C	277	-57.877	-44.673	-11.780	1.00	17.26
12630	C	GLU	C	277	-61.992	-47.744	-11.527	1.00	17.38
12631	O	GLU	C	277	-63.137	-47.319	-11.369	1.00	18.10
12632	N	PHE	C	278	-61.657	-48.528	-12.548	1.00	17.85
12634	CA	PHE	C	278	-62.648	-48.916	-13.550	1.00	18.72
12636	CB	PHE	C	278	-61.980	-49.637	-14.714	1.00	19.52
12639	CG	PHE	C	278	-62.956	-50.301	-15.631	1.00	21.01
12640	CD1	PHE	C	278	-63.693	-49.546	-16.529	1.00	24.55
12642	CE1	PHE	C	278	-64.620	-50.160	-17.365	1.00	25.63

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
12644	CZ	PHE	C	278	-64.826	-51.524	-17.279	1.00	26.02
12646	CE2	PHE	C	278	-64.111	-52.277	-16.371	1.00	25.07
12648	CD2	PHE	C	278	-63.185	-51.666	-15.550	1.00	23.74
12650	C	PHE	C	278	-63.742	-49.801	-12.936	1.00	19.15
12651	O	PHE	C	278	-64.941	-49.550	-13.115	1.00	19.58
12652	N	LEU	C	279	-63.330	-50.814	-12.192	1.00	19.14
12654	CA	LEU	C	279	-64.281	-51.784	-11.636	1.00	19.72
12656	CB	LEU	C	279	-63.547	-52.953	-10.976	1.00	19.69
12659	CG	LEU	C	279	-62.866	-53.928	-11.935	1.00	19.83
12661	CD1	LEU	C	279	-61.983	-54.880	-11.142	1.00	20.16
12665	CD2	LEU	C	279	-63.873	-54.675	-12.809	1.00	19.87
12669	C	LEU	C	279	-65.229	-51.117	-10.641	1.00	20.77
12670	O	LEU	C	279	-66.420	-51.440	-10.596	1.00	21.85
12671	N	TYR	C	280	-64.710	-50.166	-9.874	1.00	21.78
12673	CA	TYR	C	280	-65.509	-49.460	-8.875	1.00	22.98
12675	CB	TYR	C	280	-64.604	-48.657	-7.948	1.00	22.85
12678	CG	TYR	C	280	-63.756	-49.469	-6.979	1.00	20.88
12679	CD1	TYR	C	280	-62.941	-48.813	-6.057	1.00	20.74
12681	CE1	TYR	C	280	-62.160	-49.511	-5.172	1.00	21.12
12683	CZ	TYR	C	280	-62.167	-50.891	-5.178	1.00	21.71
12684	OH	TYR	C	280	-61.379	-51.564	-4.271	1.00	22.84
12686	CE2	TYR	C	280	-62.970	-51.584	-6.078	1.00	21.29
12688	CD2	TYR	C	280	-63.751	-50.872	-6.976	1.00	21.28
12690	C	TYR	C	280	-66.534	-48.536	-9.527	1.00	24.51
12691	O	TYR	C	280	-67.636	-48.375	-9.007	1.00	26.24
12692	N	SER	C	281	-66.185	-47.967	-10.674	1.00	25.25
12694	CA	SER	C	281	-67.055	-47.034	-11.383	1.00	26.30
12696	CB	SER	C	281	-66.296	-46.377	-12.543	1.00	26.33
12699	OG	SER	C	281	-66.134	-47.264	-13.640	1.00	27.98
12701	C	SER	C	281	-68.321	-47.730	-11.892	1.00	27.08
12702	O	SER	C	281	-69.340	-47.070	-12.125	1.00	28.82
12703	N	GLN	D	20	-43.213	-49.029	9.812	1.00	35.53
12705	CA	GLN	D	20	-41.978	-49.181	10.621	1.00	34.93
12707	CB	GLN	D	20	-42.035	-48.238	11.830	1.00	34.67
12710	CG	GLN	D	20	-43.417	-48.133	12.450	1.00	32.05
12713	CD	GLN	D	20	-44.329	-47.149	11.730	1.00	28.53
12714	OE1	GLN	D	20	-43.888	-46.079	11.296	1.00	21.34
12715	NE2	GLN	D	20	-45.610	-47.500	11.624	1.00	26.91
12718	C	GLN	D	20	-41.884	-50.664	10.992	1.00	35.29
12719	O	GLN	D	20	-42.195	-51.506	10.147	1.00	36.37
12723	N	GLN	D	21	-41.461	-51.004	12.209	1.00	35.37
12725	CA	GLN	D	21	-41.618	-52.379	12.691	1.00	35.30
12727	CB	GLN	D	21	-40.360	-52.881	13.419	1.00	35.55
12730	CG	GLN	D	21	-39.264	-53.490	12.512	1.00	36.15
12733	CD	GLN	D	21	-39.799	-54.154	11.237	1.00	37.29
12734	OE1	GLN	D	21	-40.534	-55.144	11.301	1.00	38.87
12735	NE2	GLN	D	21	-39.427	-53.610	10.083	1.00	37.34
12738	C	GLN	D	21	-42.852	-52.468	13.596	1.00	34.93
12739	O	GLN	D	21	-42.872	-51.893	14.688	1.00	34.87

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
12740	N	PRO	D	22	-43.882	-53.182	13.142	1.00	34.50
12741	CA	PRO	D	22	-45.117	-53.318	13.919	1.00	34.20
12743	CB	PRO	D	22	-46.113	-53.885	12.899	1.00	34.39
12746	CG	PRO	D	22	-45.277	-54.629	11.907	1.00	34.47
12749	CD	PRO	D	22	-43.940	-53.944	11.878	1.00	34.59
12752	C	PRO	D	22	-44.918	-54.284	15.084	1.00	33.99
12753	O	PRO	D	22	-44.163	-55.248	14.943	1.00	33.57
12754	N	LEU	D	23	-45.562	-54.014	16.215	1.00	33.52
12756	CA	LEU	D	23	-45.477	-54.887	17.379	1.00	33.55
12758	CB	LEU	D	23	-46.300	-54.320	18.543	1.00	33.47
12761	CG	LEU	D	23	-45.854	-52.979	19.139	1.00	33.62
12763	CD1	LEU	D	23	-46.713	-52.638	20.354	1.00	33.83
12767	CD2	LEU	D	23	-44.373	-52.988	19.510	1.00	33.97
12771	C	LEU	D	23	-45.981	-56.282	17.023	1.00	33.51
12772	O	LEU	D	23	-47.090	-56.429	16.503	1.00	33.57
12773	N	ASN	D	24	-45.159	-57.294	17.300	1.00	33.61
12775	CA	ASN	D	24	-45.513	-58.686	17.024	1.00	33.72
12777	CB	ASN	D	24	-44.250	-59.513	16.748	1.00	33.80
12780	CG	ASN	D	24	-44.561	-60.944	16.332	1.00	34.30
12781	OD1	ASN	D	24	-45.577	-61.216	15.686	1.00	35.34
12782	ND2	ASN	D	24	-43.685	-61.868	16.707	1.00	34.97
12785	C	ASN	D	24	-46.319	-59.280	18.181	1.00	33.42
12786	O	ASN	D	24	-45.826	-60.102	18.951	1.00	33.61
12787	N	GLU	D	25	-47.568	-58.842	18.291	1.00	33.03
12789	CA	GLU	D	25	-48.471	-59.299	19.342	1.00	32.66
12791	CB	GLU	D	25	-48.037	-58.756	20.711	1.00	32.96
12794	CG	GLU	D	25	-47.907	-57.242	20.786	1.00	34.33
12797	CD	GLU	D	25	-47.061	-56.784	21.962	1.00	36.12
12798	OE1	GLU	D	25	-46.065	-56.059	21.747	1.00	38.25
12799	OE2	GLU	D	25	-47.388	-57.148	23.108	1.00	38.35
12800	C	GLU	D	25	-49.903	-58.868	19.029	1.00	31.73
12801	O	GLU	D	25	-50.124	-57.905	18.294	1.00	31.53
12802	N	GLU	D	26	-50.874	-59.589	19.579	1.00	30.53
12804	CA	GLU	D	26	-52.275	-59.235	19.382	1.00	29.77
12806	CB	GLU	D	26	-53.200	-60.407	19.747	1.00	30.39
12809	CG	GLU	D	26	-53.310	-61.477	18.665	1.00	32.33
12812	CD	GLU	D	26	-54.023	-60.988	17.412	1.00	35.21
12813	OE1	GLU	D	26	-55.215	-60.611	17.502	1.00	36.80
12814	OE2	GLU	D	26	-53.390	-60.975	16.329	1.00	37.60
12815	C	GLU	D	26	-52.610	-57.995	20.210	1.00	28.32
12816	O	GLU	D	26	-52.026	-57.762	21.274	1.00	27.63
12817	N	PHE	D	27	-53.536	-57.188	19.704	1.00	26.58
12819	CA	PHE	D	27	-53.969	-55.991	20.406	1.00	25.53
12821	CB	PHE	D	27	-54.939	-55.173	19.556	1.00	25.06
12824	CG	PHE	D	27	-55.487	-53.963	20.265	1.00	23.00
12825	CD1	PHE	D	27	-54.723	-52.808	20.377	1.00	21.55
12827	CE1	PHE	D	27	-55.213	-51.692	21.031	1.00	20.67
12829	CZ	PHE	D	27	-56.486	-51.720	21.589	1.00	21.35
12831	CE2	PHE	D	27	-57.253	-52.867	21.492	1.00	22.05

## FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
12833	CD2	PHE	D	27	-56.755	-53.984	20.839	1.00	22.19
12835	C	PHE	D	27	-54.663	-56.366	21.704	1.00	25.18
12836	O	PHE	D	27	-55.423	-57.338	21.755	1.00	24.81
12837	N	ARG	D	28	-54.383	-55.589	22.743	1.00	24.90
12839	CA	ARG	D	28	-55.113	-55.654	24.004	1.00	24.81
12841	CB	ARG	D	28	-54.241	-56.255	25.102	1.00	24.97
12844	CG	ARG	D	28	-53.614	-57.600	24.744	1.00	26.25
12847	CD	ARG	D	28	-52.670	-58.146	25.807	1.00	27.58
12850	NE	BARG	D	28	-51.515	-57.265	26.015	0.35	27.81
12851	NE	AARG	D	28	-51.546	-57.244	26.064	0.65	28.63
12854	CZ	BARG	D	28	-51.260	-56.560	27.120	0.35	27.67
12855	CZ	AARG	D	28	-50.467	-57.126	25.291	0.65	28.72
12856	NH1	BARG	D	28	-52.070	-56.602	28.177	0.35	27.83
12857	NH1	AARG	D	28	-50.330	-57.859	24.186	0.65	29.18
12862	NH2	BARG	D	28	-50.172	-55.799	27.170	0.35	27.42
12863	NH2	AARG	D	28	-49.513	-56.267	25.628	0.65	29.24
12868	C	ARG	D	28	-55.513	-54.226	24.376	1.00	24.36
12869	O	ARG	D	28	-54.708	-53.308	24.211	1.00	23.52
12870	N	PRO	D	29	-56.736	-54.027	24.869	1.00	24.25
12871	CA	PRO	D	29	-57.178	-52.683	25.275	1.00	24.18
12873	CB	PRO	D	29	-58.615	-52.903	25.774	1.00	24.40
12876	CG	PRO	D	29	-58.769	-54.372	25.968	1.00	24.63
12879	CD	PRO	D	29	-57.792	-55.040	25.061	1.00	24.44
12882	C	PRO	D	29	-56.300	-52.034	26.355	1.00	23.87
12883	O	PRO	D	29	-56.269	-50.804	26.443	1.00	23.79
12884	N	GLU	D	30	-55.585	-52.848	27.134	1.00	23.67
12886	CA	GLU	D	30	-54.693	-52.361	28.188	1.00	23.57
12888	CB	GLU	D	30	-54.186	-53.529	29.045	1.00	23.93
12891	CG	GLU	D	30	-55.229	-54.118	29.984	1.00	25.91
12894	CD	GLU	D	30	-56.134	-55.163	29.346	1.00	27.74
12895	OE1	GLU	D	30	-57.090	-55.595	30.034	1.00	30.26
12896	OE2	GLU	D	30	-55.906	-55.562	28.180	1.00	26.91
12897	C	GLU	D	30	-53.497	-51.587	27.635	1.00	22.81
12898	O	GLU	D	30	-52.860	-50.834	28.363	1.00	22.79
12899	N	MET	D	31	-53.200	-51.782	26.351	1.00	22.23
12901	CA	MET	D	31	-52.141	-51.047	25.661	1.00	21.45
12903	CB	MET	D	31	-52.022	-51.525	24.210	1.00	21.52
12906	CG	MET	D	31	-51.484	-52.934	24.050	1.00	21.00
12909	SD	MET	D	31	-51.453	-53.400	22.306	1.00	20.72
12910	CE	MET	D	31	-50.291	-54.786	22.343	1.00	21.39
12914	C	MET	D	31	-52.370	-49.533	25.656	1.00	20.96
12915	O	MET	D	31	-51.422	-48.769	25.498	1.00	21.26
12916	N	LEU	D	32	-53.625	-49.112	25.792	1.00	20.36
12918	CA	LEU	D	32	-53.978	-47.692	25.806	1.00	20.12
12920	CB	LEU	D	32	-55.245	-47.447	24.969	1.00	20.35
12923	CG	LEU	D	32	-55.058	-47.222	23.458	1.00	20.52
12925	CD1	LEU	D	32	-54.493	-48.472	22.793	1.00	21.37
12929	CD2	LEU	D	32	-54.178	-46.008	23.181	1.00	21.68
12933	C	LEU	D	32	-54.197	-47.167	27.224	1.00	19.78

## FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
12934	O	LEU	D	32	-54.412	-45.982	27.417	1.00	19.56
12935	N	GLN	D	33	-54.152	-48.047	28.219	1.00	19.69
12937	CA	GLN	D	33	-54.401	-47.637	29.596	1.00	19.88
12939	CB	GLN	D	33	-54.389	-48.861	30.509	1.00	20.14
12942	CG	GLN	D	33	-55.053	-48.665	31.834	1.00	22.57
12945	CD	GLN	D	33	-55.217	-49.984	32.561	1.00	25.03
12946	OE1	GLN	D	33	-56.333	-50.485	32.711	1.00	27.96
12947	NE2	GLN	D	33	-54.101	-50.568	32.983	1.00	27.57
12950	C	GLN	D	33	-53.353	-46.630	30.060	1.00	19.21
12951	O	GLN	D	33	-52.160	-46.901	30.000	1.00	19.74
12952	N	GLY	D	34	-53.802	-45.451	30.480	1.00	18.80
12954	CA	GLY	D	34	-52.910	-44.407	30.958	1.00	18.55
12957	C	GLY	D	34	-52.144	-43.667	29.878	1.00	18.12
12958	O	GLY	D	34	-51.325	-42.801	30.185	1.00	18.38
12959	N	LYS	D	35	-52.401	-44.000	28.615	1.00	17.40
12961	CA	LYS	D	35	-51.736	-43.330	27.504	1.00	17.08
12963	CB	LYS	D	35	-51.801	-44.179	26.231	1.00	17.28
12966	CG	LYS	D	35	-51.079	-45.515	26.337	1.00	18.28
12969	CD	LYS	D	35	-49.587	-45.340	26.554	1.00	20.33
12972	CE	LYS	D	35	-48.887	-46.665	26.760	1.00	22.38
12975	NZ	LYS	D	35	-47.484	-46.443	27.215	1.00	24.78
12979	C	LYS	D	35	-52.372	-41.969	27.269	1.00	16.45
12980	O	LYS	D	35	-53.555	-41.771	27.520	1.00	17.02
12981	N	LYS	D	36	-51.568	-41.042	26.765	1.00	15.85
12983	CA	LYS	D	36	-51.960	-39.653	26.608	1.00	15.43
12985	CB	LYS	D	36	-50.847	-38.748	27.139	1.00	15.49
12988	CG	LYS	D	36	-50.626	-38.925	28.653	1.00	16.39
12991	CD	LYS	D	36	-49.262	-38.453	29.106	1.00	18.44
12994	CE	LYS	D	36	-49.045	-38.837	30.566	1.00	20.24
12997	NZ	LYS	D	36	-47.824	-38.208	31.135	1.00	22.80
13001	C	LYS	D	36	-52.214	-39.414	25.138	1.00	15.40
13002	O	LYS	D	36	-51.291	-39.487	24.347	1.00	15.35
13003	N	VAL	D	37	-53.465	-39.159	24.779	1.00	14.89
13005	CA	VAL	D	37	-53.872	-39.149	23.376	1.00	14.49
13007	CB	VAL	D	37	-54.729	-40.385	23.037	1.00	14.54
13009	CG1	VAL	D	37	-54.947	-40.490	21.524	1.00	15.16
13013	CG2	VAL	D	37	-54.083	-41.655	23.578	1.00	15.88
13017	C	VAL	D	37	-54.650	-37.895	22.983	1.00	14.45
13018	O	VAL	D	37	-55.582	-37.485	23.671	1.00	14.07
13019	N	ILE	D	38	-54.246	-37.293	21.867	1.00	14.15
13021	CA	ILE	D	38	-54.984	-36.213	21.219	1.00	14.29
13023	CB	ILE	D	38	-54.008	-35.189	20.602	1.00	14.22
13025	CG1	ILE	D	38	-53.410	-34.294	21.692	1.00	14.47
13028	CD1	ILE	D	38	-52.240	-33.464	21.208	1.00	13.47
13032	CG2	ILE	D	38	-54.694	-34.353	19.479	1.00	13.72
13036	C	ILE	D	38	-55.823	-36.835	20.119	1.00	14.66
13037	O	ILE	D	38	-55.313	-37.652	19.346	1.00	14.40
13038	N	VAL	D	39	-57.093	-36.446	20.043	1.00	14.41
13040	CA	VAL	D	39	-57.940	-36.792	18.901	1.00	14.71

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
13042	CB	VAL	D	39	-59.115	-37.704	19.289	1.00	14.96
13044	CG1	VAL	D	39	-59.796	-38.237	18.030	1.00	15.66
13048	CG2	VAL	D	39	-58.638	-38.832	20.178	1.00	15.63
13052	C	VAL	D	39	-58.490	-35.502	18.309	1.00	14.26
13053	O	VAL	D	39	-59.143	-34.727	19.001	1.00	14.39
13054	N	THR	D	40	-58.216	-35.250	17.032	1.00	13.79
13056	CA	THR	D	40	-58.815	-34.097	16.374	1.00	13.70
13058	CB	THR	D	40	-57.830	-33.372	15.443	1.00	13.33
13060	OG1	THR	D	40	-57.631	-34.126	14.240	1.00	14.34
13062	CG2	THR	D	40	-56.455	-33.245	16.047	1.00	13.29
13066	C	THR	D	40	-60.057	-34.532	15.609	1.00	13.41
13067	O	THR	D	40	-60.292	-35.722	15.390	1.00	13.63
13068	N	GLY	D	41	-60.853	-33.556	15.210	1.00	13.42
13070	CA	GLY	D	41	-62.152	-33.813	14.620	1.00	14.27
13073	C	GLY	D	41	-62.972	-34.779	15.449	1.00	14.75
13074	O	GLY	D	41	-63.550	-35.712	14.906	1.00	15.02
13075	N	ALA	D	42	-63.043	-34.527	16.759	1.00	15.40
13077	CA	ALA	D	42	-63.594	-35.478	17.729	1.00	15.81
13079	CB	ALA	D	42	-62.605	-35.659	18.855	1.00	16.55
13083	C	ALA	D	42	-64.981	-35.129	18.295	1.00	16.04
13084	O	ALA	D	42	-65.448	-35.773	19.239	1.00	16.36
13085	N	SER	D	43	-65.640	-34.128	17.726	1.00	16.06
13087	CA	SER	D	43	-66.986	-33.747	18.165	1.00	16.28
13089	CB	SER	D	43	-67.280	-32.308	17.765	1.00	16.60
13092	OG	SER	D	43	-67.218	-32.140	16.361	1.00	16.23
13094	C	SER	D	43	-68.083	-34.661	17.605	1.00	16.50
13095	O	SER	D	43	-69.197	-34.711	18.143	1.00	16.79
13096	N	LYS	D	44	-67.788	-35.339	16.498	1.00	15.89
13098	CA	LYS	D	44	-68.731	-36.259	15.868	1.00	15.95
13100	CB	LYS	D	44	-69.754	-35.486	15.032	1.00	16.60
13103	CG	LYS	D	44	-69.176	-34.691	13.867	1.00	17.76
13106	CD	LYS	D	44	-70.256	-33.846	13.187	1.00	19.81
13109	CE	LYS	D	44	-69.735	-33.132	11.949	1.00	21.72
13112	NZ	LYS	D	44	-70.765	-32.221	11.366	1.00	23.31
13116	C	LYS	D	44	-67.987	-37.287	15.006	1.00	15.31
13117	O	LYS	D	44	-66.756	-37.295	14.979	1.00	14.54
13118	N	GLY	D	45	-68.739	-38.174	14.356	1.00	15.02
13120	CA	GLY	D	45	-68.172	-39.125	13.405	1.00	15.06
13123	C	GLY	D	45	-67.183	-40.094	14.024	1.00	14.94
13124	O	GLY	D	45	-67.291	-40.477	15.197	1.00	15.10
13125	N	ILE	D	46	-66.205	-40.497	13.223	1.00	14.50
13127	CA	ILE	D	46	-65.190	-41.444	13.651	1.00	14.49
13129	CB	ILE	D	46	-64.298	-41.834	12.440	1.00	14.34
13131	CG1	ILE	D	46	-65.152	-42.521	11.369	1.00	14.52
13134	CD1	ILE	D	46	-64.619	-42.340	9.962	1.00	15.30
13138	CG2	ILE	D	46	-63.172	-42.759	12.854	1.00	15.39
13142	C	ILE	D	46	-64.362	-40.902	14.819	1.00	14.22
13143	O	ILE	D	46	-64.015	-41.648	15.725	1.00	14.26
13144	N	GLY	D	47	-64.062	-39.605	14.798	1.00	14.29

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
13146	CA	GLY	D	47	-63.269	-38.971	15.836	1.00	14.10
13149	C	GLY	D	47	-63.913	-39.107	17.209	1.00	14.14
13150	O	GLY	D	47	-63.254	-39.467	18.178	1.00	14.08
13151	N	ARG	D	48	-65.207	-38.816	17.277	1.00	14.17
13153	CA	ARG	D	48	-65.954	-38.994	18.528	1.00	14.45
13155	CB	ARG	D	48	-67.413	-38.587	18.337	1.00	14.52
13158	CG	ARG	D	48	-68.269	-38.703	19.591	1.00	16.48
13161	CD	ARG	D	48	-69.612	-38.029	19.458	1.00	18.45
13164	NE	ARG	D	48	-70.364	-38.565	18.326	1.00	21.04
13166	CZ	ARG	D	48	-71.458	-38.012	17.815	1.00	23.54
13167	NH1	ARG	D	48	-71.977	-36.909	18.349	1.00	25.29
13170	NH2	ARG	D	48	-72.052	-38.574	16.766	1.00	24.30
13173	C	ARG	D	48	-65.885	-40.443	19.002	1.00	14.84
13174	O	ARG	D	48	-65.648	-40.695	20.184	1.00	15.19
13175	N	GLU	D	49	-66.110	-41.387	18.093	1.00	14.91
13177	CA	GLU	D	49	-66.038	-42.811	18.438	1.00	15.16
13179	CB	GLU	D	49	-66.484	-43.696	17.268	1.00	15.73
13182	CG	GLU	D	49	-67.925	-43.500	16.802	1.00	17.94
13185	CD	GLU	D	49	-68.955	-43.646	17.908	1.00	21.21
13186	OE1	GLU	D	49	-69.940	-42.870	17.923	1.00	22.92
13187	OE2	GLU	D	49	-68.790	-44.539	18.759	1.00	23.86
13188	C	GLU	D	49	-64.651	-43.242	18.910	1.00	14.85
13189	O	GLU	D	49	-64.539	-44.119	19.758	1.00	14.65
13190	N	MET	D	50	-63.596	-42.638	18.362	1.00	14.23
13192	CA	MET	D	50	-62.235	-42.926	18.815	1.00	14.22
13194	CB	MET	D	50	-61.187	-42.342	17.864	1.00	14.64
13197	CG	MET	D	50	-61.053	-43.142	16.593	1.00	14.82
13200	SD	MET	D	50	-59.683	-42.626	15.549	1.00	15.26
13201	CE	MET	D	50	-60.229	-41.022	15.048	1.00	16.09
13205	C	MET	D	50	-62.045	-42.408	20.244	1.00	14.35
13206	O	MET	D	50	-61.486	-43.108	21.083	1.00	13.96
13207	N	ALA	D	51	-62.522	-41.199	20.524	1.00	14.65
13209	CA	ALA	D	51	-62.464	-40.661	21.888	1.00	14.97
13211	CB	ALA	D	51	-63.086	-39.281	21.950	1.00	15.27
13215	C	ALA	D	51	-63.147	-41.588	22.877	1.00	14.95
13216	O	ALA	D	51	-62.615	-41.853	23.947	1.00	15.58
13217	N	TYR	D	52	-64.313	-42.095	22.506	1.00	14.90
13219	CA	TYR	D	52	-65.067	-42.984	23.389	1.00	14.93
13221	CB	TYR	D	52	-66.468	-43.222	22.829	1.00	15.14
13224	CG	TYR	D	52	-67.398	-42.019	22.889	1.00	15.78
13225	CD1	TYR	D	52	-67.058	-40.863	23.590	1.00	15.69
13227	CE1	TYR	D	52	-67.913	-39.769	23.625	1.00	17.43
13229	CZ	TYR	D	52	-69.115	-39.822	22.970	1.00	16.96
13230	OH	TYR	D	52	-69.959	-38.734	23.036	1.00	21.07
13232	CE2	TYR	D	52	-69.485	-40.957	22.278	1.00	17.19
13234	CD2	TYR	D	52	-68.622	-42.044	22.235	1.00	17.16
13236	C	TYR	D	52	-64.348	-44.313	23.627	1.00	15.41
13237	O	TYR	D	52	-64.324	-44.805	24.750	1.00	15.63
13238	N	HIS	D	53	-63.760	-44.896	22.585	1.00	15.29



# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
13240	CA	HIS	D	53	-63.002	-46.135	22.742	1.00	15.88
13242	CB	HIS	D	53	-62.509	-46.666	21.388	1.00	15.92
13245	CG	HIS	D	53	-63.524	-47.470	20.647	1.00	17.59
13246	ND1	HIS	D	53	-64.079	-48.625	21.157	1.00	19.23
13248	CE1	HIS	D	53	-64.932	-49.123	20.280	1.00	19.57
13250	NE2	HIS	D	53	-64.947	-48.338	19.220	1.00	19.83
13252	CD2	HIS	D	53	-64.077	-47.296	19.423	1.00	19.48
13254	C	HIS	D	53	-61.808	-45.913	23.656	1.00	15.70
13255	O	HIS	D	53	-61.502	-46.751	24.496	1.00	15.89
13256	N	LEU	D	54	-61.131	-44.781	23.486	1.00	15.83
13258	CA	LEU	D	54	-59.958	-44.464	24.280	1.00	15.68
13260	CB	LEU	D	54	-59.278	-43.194	23.771	1.00	15.77
13263	CG	LEU	D	54	-58.540	-43.418	22.452	1.00	15.44
13265	CD1	LEU	D	54	-58.229	-42.078	21.791	1.00	15.31
13269	CD2	LEU	D	54	-57.262	-44.231	22.679	1.00	16.16
13273	C	LEU	D	54	-60.373	-44.290	25.730	1.00	15.87
13274	O	LEU	D	54	-59.678	-44.742	26.639	1.00	16.62
13275	N	ALA	D	55	-61.533	-43.678	25.919	1.00	16.59
13277	CA	ALA	D	55	-62.096	-43.451	27.249	1.00	17.08
13279	CB	ALA	D	55	-63.383	-42.650	27.148	1.00	17.31
13283	C	ALA	D	55	-62.351	-44.787	27.948	1.00	17.76
13284	O	ALA	D	55	-61.937	-44.978	29.086	1.00	17.71
13285	N	LYS	D	56	-62.996	-45.718	27.245	1.00	18.33
13287	CA	LYS	D	56	-63.267	-47.063	27.769	1.00	19.06
13289	CB	LYS	D	56	-64.063	-47.881	26.748	1.00	19.43
13292	CG	LYS	D	56	-65.515	-47.470	26.606	1.00	22.17
13295	CD	LYS	D	56	-66.254	-48.340	25.588	1.00	25.20
13298	CE	LYS	D	56	-67.682	-47.836	25.388	1.00	27.07
13301	NZ	LYS	D	56	-68.540	-48.779	24.609	1.00	28.97
13305	C	LYS	D	56	-61.988	-47.825	28.131	1.00	19.01
13306	O	LYS	D	56	-61.987	-48.648	29.049	1.00	19.09
13307	N	MET	D	57	-60.906	-47.553	27.405	1.00	18.87
13309	CA	MET	D	57	-59.606	-48.174	27.663	1.00	18.94
13311	CB	MET	D	57	-58.767	-48.195	26.380	1.00	19.22
13314	CG	MET	D	57	-59.347	-49.060	25.285	1.00	20.67
13317	SD	MET	D	57	-58.430	-48.919	23.737	1.00	25.77
13318	CE	MET	D	57	-59.684	-49.364	22.550	1.00	25.96
13322	C	MET	D	57	-58.813	-47.489	28.788	1.00	18.40
13323	O	MET	D	57	-57.730	-47.941	29.149	1.00	18.23
13324	N	GLY	D	58	-59.337	-46.393	29.331	1.00	17.89
13326	CA	GLY	D	58	-58.696	-45.709	30.444	1.00	17.48
13329	C	GLY	D	58	-57.554	-44.804	30.031	1.00	17.04
13330	O	GLY	D	58	-56.611	-44.593	30.792	1.00	16.65
13331	N	ALA	D	59	-57.632	-44.269	28.815	1.00	16.84
13333	CA	ALA	D	59	-56.649	-43.308	28.348	1.00	16.40
13335	CB	ALA	D	59	-56.627	-43.276	26.821	1.00	16.37
13339	C	ALA	D	59	-56.951	-41.915	28.885	1.00	16.52
13340	O	ALA	D	59	-58.061	-41.638	29.345	1.00	16.65
13341	N	HIS	D	60	-55.935	-41.059	28.841	1.00	16.33

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
13343	CA	HIS	D	60	-56.117	-39.622	28.970	1.00	16.43
13345	CB	HIS	D	60	-54.853	-38.962	29.493	1.00	16.81
13348	CG	HIS	D	60	-54.433	-39.419	30.851	1.00	17.95
13349	ND1	HIS	D	60	-54.571	-38.627	31.969	1.00	20.59
13351	CE1	HIS	D	60	-54.094	-39.268	33.019	1.00	20.83
13353	NE2	HIS	D	60	-53.653	-40.449	32.626	1.00	21.30
13355	CD2	HIS	D	60	-53.846	-40.564	31.269	1.00	19.18
13357	C	HIS	D	60	-56.374	-39.082	27.577	1.00	16.45
13358	O	HIS	D	60	-55.618	-39.398	26.656	1.00	15.81
13359	N	VAL	D	61	-57.416	-38.278	27.412	1.00	16.32
13361	CA	VAL	D	61	-57.748	-37.751	26.090	1.00	16.73
13363	CB	VAL	D	61	-59.011	-38.418	25.476	1.00	17.29
13365	CG1	VAL	D	61	-58.870	-39.942	25.475	1.00	18.64
13369	CG2	VAL	D	61	-60.268	-38.012	26.200	1.00	17.82
13373	C	VAL	D	61	-57.914	-36.246	26.114	1.00	16.32
13374	O	VAL	D	61	-58.416	-35.681	27.078	1.00	15.58
13375	N	VAL	D	62	-57.435	-35.603	25.057	1.00	15.37
13377	CA	VAL	D	62	-57.749	-34.214	24.758	1.00	15.64
13379	CB	VAL	D	62	-56.513	-33.296	24.819	1.00	15.33
13381	CG1	VAL	D	62	-56.881	-31.873	24.407	1.00	15.18
13385	CG2	VAL	D	62	-55.901	-33.297	26.227	1.00	16.56
13389	C	VAL	D	62	-58.350	-34.204	23.359	1.00	15.53
13390	O	VAL	D	62	-57.717	-34.655	22.391	1.00	16.35
13391	N	VAL	D	63	-59.584	-33.723	23.268	1.00	15.31
13393	CA	VAL	D	63	-60.319	-33.693	22.016	1.00	15.13
13395	CB	VAL	D	63	-61.727	-34.322	22.157	1.00	15.50
13397	CG1	VAL	D	63	-62.531	-33.647	23.253	1.00	16.05
13401	CG2	VAL	D	63	-61.622	-35.820	22.417	1.00	15.61
13405	C	VAL	D	63	-60.407	-32.265	21.509	1.00	15.30
13406	O	VAL	D	63	-60.385	-31.306	22.289	1.00	15.00
13407	N	THR	D	64	-60.486	-32.124	20.193	1.00	14.80
13409	CA	THR	D	64	-60.665	-30.820	19.584	1.00	14.93
13411	CB	THR	D	64	-59.286	-30.148	19.304	1.00	15.17
13413	OG1	THR	D	64	-59.465	-28.805	18.826	1.00	14.85
13415	CG2	THR	D	64	-58.520	-30.860	18.199	1.00	14.72
13419	C	THR	D	64	-61.560	-30.910	18.350	1.00	15.11
13420	O	THR	D	64	-61.747	-31.987	17.765	1.00	15.38
13421	N	ALA	D	65	-62.139	-29.755	18.035	1.00	14.88
13423	CA	ALA	D	65	-63.042	-29.487	16.912	1.00	15.56
13425	CB	ALA	D	65	-64.260	-30.383	16.933	1.00	15.43
13429	C	ALA	D	65	-63.436	-28.022	17.119	1.00	16.24
13430	O	ALA	D	65	-62.909	-27.378	18.017	1.00	16.32
13431	N	ARG	D	66	-64.360	-27.495	16.328	1.00	17.07
13433	CA	ARG	D	66	-64.681	-26.068	16.427	1.00	18.47
13435	CB	ARG	D	66	-65.158	-25.510	15.092	1.00	18.10
13438	CG	ARG	D	66	-64.067	-25.449	14.028	1.00	17.70
13441	CD	ARG	D	66	-64.594	-25.105	12.649	1.00	18.24
13444	NE	ARG	D	66	-65.542	-26.119	12.192	1.00	18.56
13446	CZ	ARG	D	66	-66.310	-26.010	11.120	1.00	18.54

## FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
13447	NH1	ARG	D	66	-67.146	-26.994	10.819	1.00	19.00
13450	NH2	ARG	D	66	-66.234	-24.944	10.328	1.00	20.56
13453	C	ARG	D	66	-65.735	-25.782	17.488	1.00	20.21
13454	O	ARG	D	66	-65.750	-24.686	18.057	1.00	20.65
13455	N	SER	D	67	-66.607	-26.758	17.737	1.00	22.28
13457	CA	SER	D	67	-67.815	-26.541	18.541	1.00	24.10
13459	CB	SER	D	67	-68.975	-27.341	17.947	1.00	24.32
13462	OG	SER	D	67	-70.126	-27.269	18.768	1.00	26.98
13464	C	SER	D	67	-67.616	-26.925	20.005	1.00	25.02
13465	O	SER	D	67	-67.574	-28.104	20.338	1.00	25.05
13466	N	LYS	D	68	-67.507	-25.922	20.872	1.00	25.92
13468	CA	LYS	D	68	-67.275	-26.153	22.297	1.00	26.88
13470	CB	LYS	D	68	-66.959	-24.837	23.027	1.00	27.37
13473	CG	LYS	D	68	-68.146	-23.895	23.209	1.00	29.09
13476	CD	LYS	D	68	-67.703	-22.453	23.458	1.00	30.27
13479	CE	LYS	D	68	-68.730	-21.445	22.932	1.00	31.55
13482	NZ	LYS	D	68	-68.798	-20.217	23.778	1.00	31.94
13486	C	LYS	D	68	-68.444	-26.875	22.969	1.00	26.67
13487	O	LYS	D	68	-68.230	-27.670	23.876	1.00	26.79
13488	N	GLU	D	69	-69.666	-26.613	22.511	1.00	26.67
13490	CA	GLU	D	69	-70.856	-27.231	23.095	1.00	26.60
13492	CB	GLU	D	69	-72.136	-26.647	22.480	1.00	27.13
13495	CG	GLU	D	69	-72.463	-25.228	22.933	1.00	28.84
13498	CD	GLU	D	69	-71.828	-24.141	22.079	1.00	30.87
13499	OE1	GLU	D	69	-72.010	-22.951	22.421	1.00	32.20
13500	OE2	GLU	D	69	-71.148	-24.460	21.072	1.00	32.91
13501	C	GLU	D	69	-70.843	-28.744	22.900	1.00	26.03
13502	O	GLU	D	69	-71.096	-29.503	23.845	1.00	25.84
13503	N	THR	D	70	-70.552	-29.170	21.672	1.00	24.98
13505	CA	THR	D	70	-70.530	-30.591	21.333	1.00	24.44
13507	CB	THR	D	70	-70.556	-30.818	19.803	1.00	24.55
13509	OG1	THR	D	70	-69.490	-30.099	19.163	1.00	26.54
13511	CG2	THR	D	70	-71.821	-30.240	19.190	1.00	23.88
13515	C	THR	D	70	-69.323	-31.270	21.958	1.00	23.28
13516	O	THR	D	70	-69.424	-32.402	22.405	1.00	23.33
13517	N	LEU	D	71	-68.192	-30.568	22.007	1.00	21.87
13519	CA	LEU	D	71	-66.982	-31.107	22.623	1.00	21.18
13521	CB	LEU	D	71	-65.787	-30.171	22.412	1.00	20.87
13524	CG	LEU	D	71	-65.157	-30.163	21.014	1.00	20.02
13526	CD1	LEU	D	71	-64.173	-29.013	20.898	1.00	19.62
13530	CD2	LEU	D	71	-64.466	-31.501	20.710	1.00	19.65
13534	C	LEU	D	71	-67.171	-31.342	24.118	1.00	21.23
13535	O	LEU	D	71	-66.643	-32.302	24.662	1.00	20.60
13536	N	GLN	D	72	-67.908	-30.452	24.780	1.00	21.21
13538	CA	GLN	D	72	-68.179	-30.609	26.206	1.00	21.75
13540	CB	GLN	D	72	-68.926	-29.390	26.764	1.00	22.00
13543	CG	GLN	D	72	-69.338	-29.524	28.231	1.00	23.59
13546	CD	GLN	D	72	-68.156	-29.781	29.152	1.00	25.57
13547	OE1	GLN	D	72	-67.368	-28.871	29.414	1.00	28.46

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
13548	NE2	GLN	D	72	-68.030	-31.016	29.646	1.00	26.08
13551	C	GLN	D	72	-68.984	-31.882	26.453	1.00	21.39
13552	O	GLN	D	72	-68.756	-32.575	27.445	1.00	21.80
13553	N	LYS	D	73	-69.923	-32.179	25.554	1.00	21.16
13555	CA	LYS	D	73	-70.725	-33.396	25.653	1.00	21.14
13557	CB	LYS	D	73	-71.868	-33.393	24.633	1.00	21.82
13560	CG	LYS	D	73	-72.862	-32.248	24.819	1.00	23.90
13563	CD	LYS	D	73	-74.236	-32.595	24.263	1.00	26.55
13566	CE	LYS	D	73	-75.224	-31.462	24.461	1.00	27.92
13569	NZ	LYS	D	73	-76.606	-31.980	24.674	1.00	29.70
13573	C	LYS	D	73	-69.857	-34.638	25.463	1.00	20.40
13574	O	LYS	D	73	-70.064	-35.647	26.133	1.00	20.36
13575	N	VAL	D	74	-68.879	-34.558	24.560	1.00	19.26
13577	CA	VAL	D	74	-67.978	-35.675	24.328	1.00	18.61
13579	CB	VAL	D	74	-67.115	-35.463	23.049	1.00	18.14
13581	CG1	VAL	D	74	-65.993	-36.494	22.958	1.00	18.71
13585	CG2	VAL	D	74	-68.010	-35.543	21.833	1.00	18.61
13589	C	VAL	D	74	-67.099	-35.901	25.550	1.00	18.35
13590	O	VAL	D	74	-66.912	-37.039	25.967	1.00	18.87
13591	N	VAL	D	75	-66.576	-34.823	26.129	1.00	18.41
13593	CA	VAL	D	75	-65.720	-34.922	27.309	1.00	18.43
13595	CB	VAL	D	75	-65.123	-33.543	27.721	1.00	18.32
13597	CG1	VAL	D	75	-64.061	-33.105	26.710	1.00	18.96
13601	CG2	VAL	D	75	-64.512	-33.586	29.114	1.00	18.56
13605	C	VAL	D	75	-66.502	-35.557	28.460	1.00	18.60
13606	O	VAL	D	75	-65.998	-36.451	29.124	1.00	17.68
13607	N	SER	D	76	-67.744	-35.126	28.658	1.00	19.64
13609	CA	SER	D	76	-68.556	-35.640	29.767	1.00	19.94
13611	CB	BSER	D	76	-69.884	-34.882	29.867	0.35	19.93
13612	CB	ASER	D	76	-69.878	-34.875	29.896	0.65	20.22
13617	OG	BSER	D	76	-69.673	-33.529	30.218	0.35	19.26
13618	OG	ASER	D	76	-70.597	-35.319	31.036	0.65	21.86
13621	C	SER	D	76	-68.826	-37.137	29.602	1.00	20.12
13622	O	SER	D	76	-68.837	-37.882	30.586	1.00	20.15
13623	N	HIS	D	77	-69.035	-37.582	28.365	1.00	20.16
13625	CA	HIS	D	77	-69.263	-38.998	28.113	1.00	20.05
13627	CB	HIS	D	77	-69.866	-39.247	26.730	1.00	20.07
13630	CG	HIS	D	77	-70.517	-40.591	26.595	1.00	21.08
13631	ND1	HIS	D	77	-70.131	-41.521	25.652	1.00	23.13
13633	CE1	HIS	D	77	-70.878	-42.604	25.770	1.00	23.08
13635	NE2	HIS	D	77	-71.729	-42.415	26.763	1.00	23.44
13637	CD2	HIS	D	77	-71.520	-41.168	27.298	1.00	22.18
13639	C	HIS	D	77	-67.977	-39.798	28.292	1.00	19.84
13640	O	HIS	D	77	-68.013	-40.899	28.819	1.00	19.65
13641	N	CYS	D	78	-66.845	-39.241	27.858	1.00	19.41
13643	CA	CYS	D	78	-65.544	-39.882	28.059	1.00	19.28
13645	CB	CYS	D	78	-64.411	-39.024	27.486	1.00	19.16
13648	SG	CYS	D	78	-64.314	-39.059	25.677	1.00	19.2
13649	C	CYS	D	78	-65.292	-40.161	29.547	1.00	19.56

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
13650	O	CYS	D	78	-64.892	-41.253	29.913	1.00	19.33
13651	N	LEU	D	79	-65.559	-39.182	30.406	1.00	19.85
13653	CA	LEU	D	79	-65.372	-39.373	31.844	1.00	20.34
13655	CB	LEU	D	79	-65.592	-38.058	32.598	1.00	20.46
13658	CG	LEU	D	79	-64.540	-36.971	32.320	1.00	20.52
13660	CD1	LEU	D	79	-63.167	-37.388	32.834	1.00	20.72
13664	CD2	LEU	D	79	-64.958	-35.637	32.929	1.00	21.91
13668	C	LEU	D	79	-66.287	-40.485	32.372	1.00	20.60
13669	O	LEU	D	79	-65.846	-41.321	33.162	1.00	20.51
13670	N	GLU	D	80	-67.538	-40.515	31.909	1.00	21.00
13672	CA	GLU	D	80	-68.493	-41.562	32.306	1.00	21.67
13674	CB	GLU	D	80	-69.864	-41.317	31.665	1.00	22.31
13677	CG	GLU	D	80	-70.690	-40.210	32.291	1.00	24.78
13680	CD	GLU	D	80	-72.018	-39.991	31.577	1.00	27.49
13681	OE1	GLU	D	80	-72.041	-39.968	30.325	1.00	29.83
13682	OE2	GLU	D	80	-73.050	-39.837	32.267	1.00	30.43
13683	C	GLU	D	80	-68.022	-42.962	31.899	1.00	21.34
13684	O	GLU	D	80	-68.232	-43.934	32.617	1.00	21.40
13685	N	LEU	D	81	-67.384	-43.048	30.735	1.00	20.60
13687	CA	LEU	D	81	-66.927	-44.313	30.167	1.00	20.28
13689	CB	LEU	D	81	-66.653	-44.147	28.668	1.00	20.07
13692	CG	LEU	D	81	-67.862	-44.055	27.743	1.00	20.59
13694	CD1	LEU	D	81	-67.412	-43.691	26.324	1.00	21.10
13698	CD2	LEU	D	81	-68.651	-45.353	27.744	1.00	21.07
13702	C	LEU	D	81	-65.668	-44.855	30.827	1.00	19.71
13703	O	LEU	D	81	-65.320	-46.011	30.616	1.00	19.37
13704	N	GLY	D	82	-64.965	-44.006	31.577	1.00	19.28
13706	CA	GLY	D	82	-63.777	-44.417	32.296	1.00	19.12
13709	C	GLY	D	82	-62.462	-43.778	31.892	1.00	18.68
13710	O	GLY	D	82	-61.418	-44.306	32.242	1.00	18.69
13711	N	ALA	D	83	-62.490	-42.640	31.198	1.00	18.38
13713	CA	ALA	D	83	-61.251	-41.955	30.840	1.00	18.46
13715	CB	ALA	D	83	-61.546	-40.735	29.975	1.00	18.46
13719	C	ALA	D	83	-60.465	-41.552	32.095	1.00	18.79
13720	O	ALA	D	83	-61.050	-41.106	33.092	1.00	18.75
13721	N	ALA	D	84	-59.148	-41.742	32.048	1.00	18.64
13723	CA	ALA	D	84	-58.246	-41.319	33.122	1.00	18.68
13725	CB	ALA	D	84	-56.822	-41.714	32.800	1.00	18.67
13729	C	ALA	D	84	-58.325	-39.818	33.351	1.00	18.61
13730	O	ALA	D	84	-58.211	-39.346	34.483	1.00	18.08
13731	N	SER	D	85	-58.465	-39.088	32.251	1.00	18.01
13733	CA	SER	D	85	-58.838	-37.675	32.245	1.00	18.23
13735	CB	SER	D	85	-57.655	-36.768	32.614	1.00	18.54
13738	OG	SER	D	85	-56.655	-36.750	31.613	1.00	18.84
13740	C	SER	D	85	-59.367	-37.320	30.855	1.00	17.98
13741	O	SER	D	85	-59.109	-38.037	29.884	1.00	17.85
13742	N	ALA	D	86	-60.127	-36.234	30.762	1.00	17.77
13744	CA	ALA	D	86	-60.647	-35.776	29.477	1.00	17.26
13746	CB	ALA	D	86	-61.979	-36.443	29.172	1.00	17.29

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
13750	C	ALA	D	86	-60.800	-34.261	29.482	1.00	17.29
13751	O	ALA	D	86	-61.365	-33.696	30.413	1.00	17.23
13752	N	HIS	D	87	-60.268	-33.611	28.450	1.00	16.78
13754	CA	HIS	D	87	-60.387	-32.167	28.270	1.00	16.80
13756	CB	HIS	D	87	-59.075	-31.462	28.627	1.00	16.59
13759	CG	HIS	D	87	-58.650	-31.645	30.048	1.00	18.73
13760	ND1	HIS	D	87	-57.992	-32.774	30.491	1.00	19.97
13762	CE1	HIS	D	87	-57.757	-32.662	31.787	1.00	22.31
13764	NE2	HIS	D	87	-58.227	-31.500	32.198	1.00	22.08
13766	CD2	HIS	D	87	-58.797	-30.845	31.132	1.00	20.34
13768	C	HIS	D	87	-60.705	-31.887	26.808	1.00	16.76
13769	O	HIS	D	87	-60.474	-32.731	25.946	1.00	16.32
13770	N	TYR	D	88	-61.243	-30.707	26.537	1.00	16.44
13772	CA	TYR	D	88	-61.379	-30.227	25.167	1.00	16.99
13774	CB	TYR	D	88	-62.845	-30.187	24.735	1.00	17.08
13777	CG	TYR	D	88	-63.632	-29.017	25.296	1.00	18.69
13778	CD1	TYR	D	88	-63.718	-27.811	24.601	1.00	20.27
13780	CE1	TYR	D	88	-64.447	-26.736	25.107	1.00	22.08
13782	CZ	TYR	D	88	-65.097	-26.872	26.317	1.00	22.48
13783	OH	TYR	D	88	-65.814	-25.806	26.818	1.00	23.79
13785	CE2	TYR	D	88	-65.023	-28.056	27.025	1.00	21.58
13787	CD2	TYR	D	88	-64.297	-29.125	26.510	1.00	20.81
13789	C	TYR	D	88	-60.743	-28.851	25.014	1.00	17.05
13790	O	TYR	D	88	-60.649	-28.078	25.964	1.00	17.08
13791	N	ILE	D	89	-60.276	-28.570	23.803	1.00	17.08
13793	CA	ILE	D	89	-59.863	-27.241	23.404	1.00	17.19
13795	CB	ILE	D	89	-58.328	-27.153	23.309	1.00	17.53
13797	CG1	ILE	D	89	-57.679	-27.575	24.628	1.00	18.25
13800	CD1	ILE	D	89	-56.176	-27.649	24.589	1.00	18.53
13804	CG2	ILE	D	89	-57.892	-25.737	22.929	1.00	18.48
13808	C	ILE	D	89	-60.516	-27.003	22.047	1.00	17.51
13809	O	ILE	D	89	-60.326	-27.793	21.116	1.00	17.53
13810	N	ALA	D	90	-61.322	-25.950	21.953	1.00	17.35
13812	CA	ALA	D	90	-62.054	-25.652	20.730	1.00	17.08
13814	CB	ALA	D	90	-63.434	-25.103	21.045	1.00	17.49
13818	C	ALA	D	90	-61.288	-24.664	19.865	1.00	16.90
13819	O	ALA	D	90	-60.719	-23.684	20.352	1.00	16.95
13820	N	GLY	D	91	-61.279	-24.926	18.568	1.00	16.29
13822	CA	GLY	D	91	-60.767	-23.970	17.613	1.00	16.12
13825	C	GLY	D	91	-60.819	-24.514	16.204	1.00	15.77
13826	O	GLY	D	91	-61.174	-25.677	15.983	1.00	16.00
13827	N	THR	D	92	-60.478	-23.661	15.246	1.00	15.57
13829	CA	THR	D	92	-60.435	-24.076	13.853	1.00	14.94
13831	CB	THR	D	92	-61.139	-23.073	12.920	1.00	15.31
13833	OG1	THR	D	92	-60.926	-23.471	11.559	1.00	14.35
13835	CG2	THR	D	92	-60.536	-21.676	12.999	1.00	15.60
13839	C	THR	D	92	-59.004	-24.336	13.404	1.00	14.65
13840	O	THR	D	92	-58.096	-23.560	13.689	1.00	14.25
13841	N	MET	D	93	-58.831	-25.430	12.664	1.00	14.20

## FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
13843	CA	MET	D	93	-57.542	-25.839	12.137	1.00	14.63
13845	CB	MET	D	93	-57.517	-27.364	11.959	1.00	14.57
13848	CG	MET	D	93	-57.577	-28.104	13.301	1.00	14.89
13851	SD	MET	D	93	-56.051	-27.913	14.216	1.00	15.45
13852	CE	MET	D	93	-56.411	-28.935	15.651	1.00	16.45
13856	C	MET	D	93	-57.226	-25.097	10.833	1.00	14.56
13857	O	MET	D	93	-56.216	-25.353	10.191	1.00	15.66
13858	N	GLU	D	94	-58.087	-24.151	10.459	1.00	14.55
13860	CA	GLU	D	94	-57.730	-23.126	9.486	1.00	15.10
13862	CB	GLU	D	94	-58.931	-22.234	9.150	1.00	15.26
13865	CG	GLU	D	94	-60.085	-22.925	8.449	1.00	16.41
13868	CD	GLU	D	94	-61.372	-22.124	8.535	1.00	17.88
13869	OE1	GLU	D	94	-61.984	-22.080	9.639	1.00	19.54
13870	OE2	GLU	D	94	-61.762	-21.515	7.508	1.00	19.72
13871	C	GLU	D	94	-56.646	-22.200	10.043	1.00	15.57
13872	O	GLU	D	94	-55.917	-21.577	9.281	1.00	15.84
13873	N	ASP	D	95	-56.586	-22.086	11.370	1.00	15.53
13875	CA	ASP	D	95	-55.692	-21.153	12.057	1.00	15.74
13877	CB	ASP	D	95	-56.454	-20.537	13.238	1.00	15.71
13880	CG	ASP	D	95	-55.626	-19.572	14.063	1.00	17.06
13881	OD1	ASP	D	95	-54.406	-19.451	13.844	1.00	18.02
13882	OD2	ASP	D	95	-56.150	-18.887	14.962	1.00	18.47
13883	C	ASP	D	95	-54.465	-21.945	12.515	1.00	15.57
13884	O	ASP	D	95	-54.538	-22.712	13.466	1.00	15.78
13885	N	MET	D	96	-53.347	-21.769	11.818	1.00	15.97
13887	CA	MET	D	96	-52.138	-22.544	12.102	1.00	16.21
13889	CB	MET	D	96	-51.086	-22.355	11.009	1.00	17.18
13892	CG	MET	D	96	-51.512	-22.826	9.629	1.00	17.92
13895	SD	MET	D	96	-51.975	-24.554	9.533	1.00	20.34
13896	CE	MET	D	96	-53.605	-24.413	8.783	1.00	22.82
13900	C	MET	D	96	-51.534	-22.196	13.464	1.00	16.30
13901	O	MET	D	96	-50.843	-23.021	14.065	1.00	16.01
13902	N	THR	D	97	-51.795	-20.986	13.946	1.00	15.89
13904	CA	THR	D	97	-51.385	-20.596	15.297	1.00	16.04
13906	CB	THR	D	97	-51.566	-19.080	15.507	1.00	16.27
13908	OG1	THR	D	97	-50.646	-18.378	14.661	1.00	17.37
13910	CG2	THR	D	97	-51.172	-18.669	16.914	1.00	16.36
13914	C	THR	D	97	-52.157	-21.392	16.334	1.00	15.54
13915	O	THR	D	97	-51.578	-21.870	17.314	1.00	16.35
13916	N	PHE	D	98	-53.459	-21.555	16.123	1.00	15.63
13918	CA	PHE	D	98	-54.253	-22.409	16.990	1.00	15.59
13920	CB	PHE	D	98	-55.733	-22.440	16.597	1.00	15.65
13923	CG	PHE	D	98	-56.498	-23.500	17.327	1.00	14.79
13924	CD1	PHE	D	98	-56.770	-23.349	18.673	1.00	15.88
13926	CE1	PHE	D	98	-57.441	-24.334	19.371	1.00	15.75
13928	CZ	PHE	D	98	-57.833	-25.493	18.733	1.00	16.14
13930	CE2	PHE	D	98	-57.561	-25.663	17.395	1.00	15.88
13932	CD2	PHE	D	98	-56.885	-24.674	16.697	1.00	15.34
13934	C	PHE	D	98	-53.718	-23.841	17.004	1.00	16.04

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
13935	O	PHE	D	98	-53.608	-24.450	18.062	1.00	15.74
13936	N	ALA	D	99	-53.404	-24.383	15.832	1.00	16.14
13938	CA	ALA	D	99	-52.918	-25.756	15.748	1.00	16.27
13940	CB	ALA	D	99	-52.606	-26.131	14.295	1.00	16.29
13944	C	ALA	D	99	-51.683	-25.945	16.628	1.00	16.95
13945	O	ALA	D	99	-51.624	-26.872	17.438	1.00	16.41
13946	N	GLU	D	100	-50.714	-25.046	16.481	1.00	17.42
13948	CA	GLU	D	100	-49.481	-25.097	17.258	1.00	17.97
13950	CB	GLU	D	100	-48.543	-23.974	16.791	1.00	18.57
13953	CG	GLU	D	100	-47.147	-24.028	17.392	1.00	21.41
13956	CD	GLU	D	100	-46.230	-22.933	16.868	1.00	25.55
13957	OE1	GLU	D	100	-45.090	-22.844	17.369	1.00	28.65
13958	OE2	GLU	D	100	-46.637	-22.158	15.966	1.00	27.39
13959	C	GLU	D	100	-49.756	-24.992	18.770	1.00	17.97
13960	O	GLU	D	100	-49.285	-25.803	19.576	1.00	17.53
13961	N	GLN	D	101	-50.557	-24.007	19.152	1.00	17.22
13963	CA	GLN	D	101	-50.805	-23.731	20.568	1.00	17.19
13965	CB	GLN	D	101	-51.462	-22.357	20.736	1.00	17.57
13968	CG	GLN	D	101	-50.537	-21.212	20.365	1.00	20.00
13971	CD	GLN	D	101	-51.154	-19.839	20.562	1.00	23.21
13972	OE1	GLN	D	101	-52.359	-19.705	20.782	1.00	26.17
13973	NE2	GLN	D	101	-50.321	-18.809	20.476	1.00	25.62
13976	C	GLN	D	101	-51.664	-24.819	21.206	1.00	16.24
13977	O	GLN	D	101	-51.523	-25.111	22.389	1.00	16.90
13978	N	PHE	D	102	-52.539	-25.423	20.408	1.00	15.13
13980	CA	PHE	D	102	-53.385	-26.515	20.862	1.00	14.42
13982	CB	PHE	D	102	-54.305	-26.991	19.741	1.00	14.41
13985	CG	PHE	D	102	-54.872	-28.348	19.985	1.00	14.30
13986	CD1	PHE	D	102	-55.828	-28.535	20.964	1.00	14.86
13988	CE1	PHE	D	102	-56.347	-29.776	21.219	1.00	15.62
13990	CZ	PHE	D	102	-55.894	-30.880	20.492	1.00	15.17
13992	CE2	PHE	D	102	-54.929	-30.714	19.521	1.00	15.21
13994	CD2	PHE	D	102	-54.414	-29.453	19.270	1.00	13.96
13996	C	PHE	D	102	-52.544	-27.699	21.339	1.00	14.36
13997	O	PHE	D	102	-52.802	-28.250	22.399	1.00	14.55
13998	N	VAL	D	103	-51.551	-28.099	20.550	1.00	14.43
14000	CA	VAL	D	103	-50.729	-29.251	20.915	1.00	14.54
14002	CB	VAL	D	103	-49.761	-29.669	19.783	1.00	14.62
14004	CG1	VAL	D	103	-48.767	-30.737	20.267	1.00	14.13
14008	CG2	VAL	D	103	-50.539	-30.202	18.611	1.00	15.45
14012	C	VAL	D	103	-49.949	-28.965	22.200	1.00	14.89
14013	O	VAL	D	103	-49.857	-29.830	23.068	1.00	15.33
14014	N	ALA	D	104	-49.399	-27.756	22.319	1.00	15.40
14016	CA	ALA	D	104	-48.673	-27.359	23.532	1.00	15.59
14018	CB	ALA	D	104	-48.132	-25.945	23.414	1.00	15.70
14022	C	ALA	D	104	-49.575	-27.461	24.749	1.00	15.68
14023	O	ALA	D	104	-49.167	-28.004	25.780	1.00	16.65
14024	N	GLN	D	105	-50.798	-26.948	24.630	1.00	15.84
14026	CA	GLN	D	105	-51.720	-26.932	25.767	1.00	16.16



# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
14028	CB	GLN	D	105	-52.880	-25.949	25.522	1.00	16.58
14031	CG	GLN	D	105	-53.870	-25.802	26.685	1.00	19.37
14034	CD	GLN	D	105	-53.254	-25.230	27.952	1.00	22.86
14035	OE1	GLN	D	105	-52.132	-24.702	27.943	1.00	26.54
14036	NE2	GLN	D	105	-53.989	-25.331	29.047	1.00	25.58
14039	C	GLN	D	105	-52.237	-28.332	26.105	1.00	15.93
14040	O	GLN	D	105	-52.362	-28.685	27.282	1.00	15.68
14041	N	ALA	D	106	-52.509	-29.142	25.089	1.00	15.72
14043	CA	ALA	D	106	-52.943	-30.516	25.304	1.00	15.69
14045	CB	ALA	D	106	-53.298	-31.184	23.970	1.00	15.46
14049	C	ALA	D	106	-51.864	-31.315	26.037	1.00	15.61
14050	O	ALA	D	106	-52.159	-32.062	26.968	1.00	15.52
14051	N	GLY	D	107	-50.615	-31.145	25.617	1.00	15.87
14053	CA	GLY	D	107	-49.489	-31.791	26.268	1.00	15.87
14056	C	GLY	D	107	-49.305	-31.327	27.696	1.00	16.47
14057	O	GLY	D	107	-48.974	-32.120	28.573	1.00	16.71
14058	N	LYS	D	108	-49.515	-30.040	27.928	1.00	16.53
14060	CA	LYS	D	108	-49.420	-29.491	29.280	1.00	16.99
14062	CB	LYS	D	108	-49.570	-27.975	29.247	1.00	17.14
14065	CG	LYS	D	108	-49.506	-27.289	30.622	1.00	18.57
14068	CD	LYS	D	108	-49.473	-25.775	30.464	1.00	20.61
14071	CE	LYS	D	108	-49.082	-25.078	31.745	1.00	22.00
14074	NZ	LYS	D	108	-49.096	-23.600	31.610	1.00	23.02
14078	C	LYS	D	108	-50.482	-30.123	30.176	1.00	17.02
14079	O	LYS	D	108	-50.190	-30.547	31.299	1.00	16.65
14080	N	LEU	D	109	-51.704	-30.210	29.665	1.00	17.05
14082	CA	LEU	D	109	-52.822	-30.780	30.412	1.00	17.17
14084	CB	LEU	D	109	-54.105	-30.736	29.577	1.00	17.59
14087	CG	LEU	D	109	-55.195	-29.673	29.761	1.00	20.18
14089	CD1	LEU	D	109	-55.686	-29.180	28.413	1.00	20.71
14093	CD2	LEU	D	109	-54.825	-28.512	30.697	1.00	20.62
14097	C	LEU	D	109	-52.554	-32.228	30.824	1.00	16.97
14098	O	LEU	D	109	-52.870	-32.623	31.948	1.00	16.89
14099	N	MET	D	110	-51.968	-33.010	29.920	1.00	16.61
14101	CA	MET	D	110	-51.783	-34.447	30.154	1.00	16.50
14103	CB	MET	D	110	-52.004	-35.216	28.847	1.00	15.95
14106	CG	MET	D	110	-53.416	-35.144	28.354	1.00	15.99
14109	SD	MET	D	110	-53.740	-36.261	26.974	1.00	16.12
14110	CE	MET	D	110	-52.815	-35.492	25.620	1.00	16.49
14114	C	MET	D	110	-50.418	-34.819	30.722	1.00	16.58
14115	O	MET	D	110	-50.237	-35.935	31.187	1.00	17.47
14116	N	GLY	D	111	-49.461	-33.900	30.667	1.00	16.66
14118	CA	GLY	D	111	-48.088	-34.189	31.053	1.00	16.95
14121	C	GLY	D	111	-47.285	-34.966	30.025	1.00	16.72
14122	O	GLY	D	111	-46.437	-35.799	30.383	1.00	16.85
14123	N	GLY	D	112	-47.542	-34.686	28.747	1.00	16.47
14125	CA	GLY	D	112	-46.882	-35.367	27.646	1.00	16.63
14128	C	GLY	D	112	-47.887	-35.869	26.617	1.00	16.27
14129	O	GLY	D	112	-49.066	-35.488	26.624	1.00	16.55

## FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
14130	N	LEU	D	113	-47.414	-36.745	25.734	1.00	15.67
14132	CA	LEU	D	113	-48.199	-37.204	24.597	1.00	15.38
14134	CB	LEU	D	113	-48.138	-36.179	23.460	1.00	15.44
14137	CG	LEU	D	113	-49.065	-36.457	22.281	1.00	15.19
14139	CD1	LEU	D	113	-50.527	-36.434	22.706	1.00	14.48
14143	CD2	LEU	D	113	-48.826	-35.479	21.144	1.00	15.59
14147	C	LEU	D	113	-47.634	-38.528	24.112	1.00	14.90
14148	O	LEU	D	113	-46.440	-38.620	23.849	1.00	15.04
14149	N	ASP	D	114	-48.489	-39.548	24.052	1.00	14.98
14151	CA	ASP	D	114	-48.137	-40.860	23.505	1.00	14.95
14153	CB	ASP	D	114	-48.693	-41.966	24.395	1.00	14.96
14156	CG	ASP	D	114	-48.128	-41.916	25.801	1.00	16.24
14157	OD1	ASP	D	114	-46.896	-42.071	25.956	1.00	17.59
14158	OD2	ASP	D	114	-48.837	-41.704	26.805	1.00	16.22
14159	C	ASP	D	114	-48.650	-41.083	22.084	1.00	15.08
14160	O	ASP	D	114	-48.011	-41.776	21.301	1.00	15.37
14161	N	MET	D	115	-49.803	-40.510	21.755	1.00	14.60
14163	CA	MET	D	115	-50.426	-40.732	20.451	1.00	14.51
14165	CB	MET	D	115	-51.426	-41.893	20.523	1.00	14.83
14168	CG	MET	D	115	-52.043	-42.274	19.174	1.00	16.13
14171	SD	MET	D	115	-53.128	-43.717	19.225	1.00	18.64
14172	CE	MET	D	115	-51.918	-45.030	19.350	1.00	19.52
14176	C	MET	D	115	-51.131	-39.472	19.953	1.00	14.49
14177	O	MET	D	115	-51.891	-38.842	20.683	1.00	14.53
14178	N	LEU	D	116	-50.880	-39.131	18.692	1.00	13.51
14180	CA	LEU	D	116	-51.495	-37.985	18.048	1.00	13.60
14182	CB	LEU	D	116	-50.407	-37.093	17.447	1.00	13.85
14185	CG	LEU	D	116	-50.866	-35.872	16.655	1.00	14.68
14187	CD1	LEU	D	116	-51.563	-34.878	17.581	1.00	15.01
14191	CD2	LEU	D	116	-49.678	-35.232	15.968	1.00	15.35
14195	C	LEU	D	116	-52.392	-38.527	16.948	1.00	13.69
14196	O	LEU	D	116	-51.895	-39.059	15.963	1.00	13.69
14197	N	ILE	D	117	-53.704	-38.395	17.113	1.00	12.97
14199	CA	ILE	D	117	-54.645	-38.878	16.109	1.00	13.06
14201	CB	ILE	D	117	-55.780	-39.710	16.731	1.00	13.04
14203	CG1	ILE	D	117	-55.203	-40.897	17.516	1.00	13.59
14206	CD1	ILE	D	117	-56.268	-41.800	18.169	1.00	15.10
14210	CG2	ILE	D	117	-56.721	-40.204	15.635	1.00	14.23
14214	C	ILE	D	117	-55.190	-37.696	15.312	1.00	12.84
14215	O	ILE	D	117	-55.934	-36.854	15.811	1.00	12.34
14216	N	LEU	D	118	-54.775	-37.646	14.056	1.00	12.43
14218	CA	LEU	D	118	-55.116	-36.569	13.134	1.00	12.90
14220	CB	LEU	D	118	-53.871	-36.176	12.337	1.00	12.82
14223	CG	LEU	D	118	-52.667	-35.780	13.186	1.00	13.08
14225	CD1	LEU	D	118	-51.446	-35.518	12.301	1.00	13.89
14229	CD2	LEU	D	118	-52.976	-34.540	14.028	1.00	15.05
14233	C	LEU	D	118	-56.235	-37.032	12.207	1.00	12.92
14234	O	LEU	D	118	-56.035	-37.886	11.347	1.00	13.25
14235	N	ASN	D	119	-57.411	-36.447	12.388	1.00	12.53

## FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
14237	CA	ASN	D	119	-58.659	-36.980	11.842	1.00	12.35
14239	CB	ASN	D	119	-59.388	-37.713	12.985	1.00	12.16
14242	CG	ASN	D	119	-60.821	-38.071	12.661	1.00	12.71
14243	OD1	ASN	D	119	-61.776	-37.403	13.139	1.00	15.78
14244	ND2	ASN	D	119	-61.005	-39.120	11.880	1.00	10.86
14247	C	ASN	D	119	-59.565	-35.922	11.187	1.00	12.08
14248	O	ASN	D	119	-60.363	-36.249	10.299	1.00	12.80
14249	N	HIS	D	120	-59.447	-34.660	11.609	1.00	12.13
14251	CA	HIS	D	120	-60.312	-33.594	11.112	1.00	12.20
14253	CB	HIS	D	120	-60.073	-32.261	11.861	1.00	11.94
14256	CG	HIS	D	120	-58.673	-31.738	11.754	1.00	13.48
14257	ND1	HIS	D	120	-58.234	-30.970	10.696	1.00	16.44
14259	CE1	HIS	D	120	-56.965	-30.656	10.882	1.00	10.79
14261	NE2	HIS	D	120	-56.553	-31.222	11.996	1.00	16.77
14263	CD2	HIS	D	120	-57.602	-31.903	12.559	1.00	12.58
14265	C	HIS	D	120	-60.146	-33.355	9.617	1.00	12.03
14266	O	HIS	D	120	-59.061	-33.569	9.056	1.00	12.88
14267	N	ILE	D	121	-61.236	-32.917	8.993	1.00	12.24
14269	CA	ILE	D	121	-61.235	-32.420	7.622	1.00	12.41
14271	CB	ILE	D	121	-61.679	-33.492	6.607	1.00	12.53
14273	CG1	ILE	D	121	-63.041	-34.091	6.968	1.00	13.26
14276	CD1	ILE	D	121	-63.656	-34.978	5.872	1.00	15.56
14280	CG2	ILE	D	121	-60.624	-34.579	6.469	1.00	13.46
14284	C	ILE	D	121	-62.168	-31.233	7.507	1.00	13.36
14285	O	ILE	D	121	-63.078	-31.067	8.313	1.00	13.55
14286	N	THR	D	122	-61.951	-30.407	6.499	1.00	13.21
14288	CA	THR	D	122	-62.896	-29.347	6.193	1.00	13.44
14290	CB	THR	D	122	-62.239	-28.258	5.357	1.00	13.46
14292	OG1	THR	D	122	-63.063	-27.085	5.393	1.00	13.39
14294	CG2	THR	D	122	-62.112	-28.641	3.871	1.00	13.36
14298	C	THR	D	122	-64.130	-29.926	5.506	1.00	14.66
14299	O	THR	D	122	-64.079	-30.995	4.888	1.00	14.62
14300	N	ASN	D	123	-65.243	-29.204	5.598	1.00	15.99
14302	CA	ASN	D	123	-66.504	-29.703	5.058	1.00	18.15
14304	CB	ASN	D	123	-67.637	-28.710	5.312	1.00	18.88
14307	CG	ASN	D	123	-68.082	-28.684	6.769	1.00	22.22
14308	OD1	ASN	D	123	-67.743	-29.567	7.567	1.00	26.94
14309	ND2	ASN	D	123	-68.848	-27.657	7.126	1.00	26.64
14312	C	ASN	D	123	-66.383	-29.981	3.573	1.00	18.51
14313	O	ASN	D	123	-65.936	-29.130	2.804	1.00	18.64
14314	N	THR	D	124	-66.804	-31.184	3.194	1.00	19.79
14316	CA	THR	D	124	-66.600	-31.736	1.864	1.00	21.01
14318	CB	THR	D	124	-65.412	-32.702	1.923	1.00	21.40
14320	OG1	THR	D	124	-64.230	-31.960	2.260	1.00	22.36
14322	CG2	THR	D	124	-65.109	-33.313	0.563	1.00	22.49
14326	C	THR	D	124	-67.841	-32.500	1.415	1.00	21.32
14327	O	THR	D	124	-68.335	-33.356	2.146	1.00	22.24
14328	N	SER	D	125	-68.328	-32.186	0.217	1.00	21.37
14330	CA	SER	D	125	-69.424	-32.933	-0.399	1.00	21.33

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
14332	CB	SER	D	125	-70.709	-32.099	-0.403	1.00	21.61
14335	OG	SER	D	125	-70.544	-30.894	-1.116	1.00	23.48
14337	C	SER	D	125	-69.039	-33.366	-1.813	1.00	20.58
14338	O	SER	D	125	-67.969	-33.013	-2.315	1.00	20.88
14339	N	LEU	D	126	-69.891	-34.167	-2.439	1.00	19.07
14341	CA	LEU	D	126	-69.635	-34.631	-3.794	1.00	18.48
14343	CB	LEU	D	126	-70.367	-35.940	-4.043	1.00	18.40
14346	CG	LEU	D	126	-69.950	-37.086	-3.125	1.00	18.69
14348	CD1	LEU	D	126	-68.474	-37.425	-3.277	1.00	19.68
14352	CD2	LEU	D	126	-70.801	-38.298	-3.428	1.00	19.60
14356	C	LEU	D	126	-70.059	-33.590	-4.820	1.00	18.25
14357	O	LEU	D	126	-71.240	-33.262	-4.935	1.00	17.52
14358	N	ASN	D	127	-69.093	-33.067	-5.568	1.00	17.29
14360	CA	ASN	D	127	-69.390	-32.108	-6.618	1.00	18.27
14362	CB	ASN	D	127	-69.617	-30.709	-6.017	1.00	18.95
14365	CG	ASN	D	127	-71.103	-30.377	-5.810	1.00	22.44
14366	OD1	ASN	D	127	-71.901	-30.382	-6.757	1.00	28.21
14367	ND2	ASN	D	127	-71.475	-30.093	-4.568	1.00	25.68
14370	C	ASN	D	127	-68.269	-32.060	-7.646	1.00	17.55
14371	O	ASN	D	127	-67.106	-32.258	-7.301	1.00	16.52
14372	N	LEU	D	128	-68.621	-31.803	-8.900	1.00	17.79
14374	CA	LEU	D	128	-67.621	-31.551	-9.937	1.00	18.36
14376	CB	LEU	D	128	-68.284	-31.283	-11.288	1.00	19.01
14379	CG	LEU	D	128	-69.023	-32.445	-11.949	1.00	21.06
14381	CD1	LEU	D	128	-69.909	-31.930	-13.067	1.00	22.44
14385	CD2	LEU	D	128	-68.043	-33.459	-12.499	1.00	22.48
14389	C	LEU	D	128	-66.784	-30.347	-9.548	1.00	18.36
14390	O	LEU	D	128	-67.269	-29.421	-8.885	1.00	19.14
14391	N	PHE	D	129	-65.509	-30.383	-9.923	1.00	17.60
14393	CA	PHE	D	129	-64.633	-29.241	-9.779	1.00	17.61
14395	CB	PHE	D	129	-63.158	-29.657	-9.780	1.00	17.01
14398	CG	PHE	D	129	-62.214	-28.490	-9.713	1.00	14.85
14399	CD1	PHE	D	129	-61.925	-27.887	-8.503	1.00	15.21
14401	CE1	PHE	D	129	-61.070	-26.790	-8.456	1.00	13.72
14403	CZ	PHE	D	129	-60.512	-26.300	-9.609	1.00	13.48
14405	CE2	PHE	D	129	-60.798	-26.877	-10.810	1.00	13.88
14407	CD2	PHE	D	129	-61.640	-27.976	-10.866	1.00	14.37
14409	C	PHE	D	129	-64.866	-28.296	-10.955	1.00	18.97
14410	O	PHE	D	129	-64.684	-28.672	-12.121	1.00	19.76
14411	N	HIS	D	130	-65.278	-27.079	-10.636	1.00	19.67
14413	CA	HIS	D	130	-65.245	-25.971	-11.582	1.00	21.03
14415	CB	HIS	D	130	-66.593	-25.768	-12.272	1.00	21.47
14418	CG	HIS	D	130	-66.555	-24.737	-13.360	1.00	24.17
14419	ND1	HIS	D	130	-66.081	-25.009	-14.627	1.00	26.18
14421	CE1	HIS	D	130	-66.159	-23.917	-15.369	1.00	26.96
14423	NE2	HIS	D	130	-66.658	-22.944	-14.627	1.00	26.86
14425	CD2	HIS	D	130	-66.909	-23.429	-13.364	1.00	26.24
14427	C	HIS	D	130	-64.868	-24.695	-10.845	1.00	21.07
14428	O	HIS	D	130	-65.633	-24.202	-9.997	1.00	21.31

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
14429	N	ASP	D	131	-63.678	-24.187	-11.151	1.00	21.38
14431	CA	ASP	D	131	-63.272	-22.848	-10.765	1.00	21.66
14433	CB	ASP	D	131	-64.146	-21.835	-11.514	1.00	22.07
14436	CG	ASP	D	131	-63.534	-20.439	-11.581	1.00	24.17
14437	OD1	ASP	D	131	-62.507	-20.178	-10.914	1.00	27.10
14438	OD2	ASP	D	131	-64.030	-19.529	-12.288	1.00	27.60
14439	C	ASP	D	131	-63.396	-22.666	-9.244	1.00	20.97
14440	O	ASP	D	131	-63.834	-21.609	-8.778	1.00	22.42
14441	N	ASP	D	132	-63.089	-23.708	-8.477	1.00	19.90
14443	CA	ASP	D	132	-63.204	-23.627	-7.023	1.00	18.58
14445	CB	ASP	D	132	-64.163	-24.693	-6.480	1.00	19.09
14448	CG	ASP	D	132	-64.702	-24.344	-5.093	1.00	20.84
14449	OD1	ASP	D	132	-64.231	-23.355	-4.474	1.00	20.27
14450	OD2	ASP	D	132	-65.614	-25.005	-4.540	1.00	23.90
14451	C	ASP	D	132	-61.841	-23.712	-6.335	1.00	17.01
14452	O	ASP	D	132	-61.594	-24.600	-5.514	1.00	16.21
14453	N	ILE	D	133	-60.984	-22.744	-6.658	1.00	15.35
14455	CA	ILE	D	133	-59.670	-22.616	-6.036	1.00	14.63
14457	CB	ILE	D	133	-58.887	-21.416	-6.645	1.00	15.30
14459	CG1	ILE	D	133	-58.682	-21.600	-8.151	1.00	16.93
14462	CD1	ILE	D	133	-57.818	-22.779	-8.516	1.00	18.50
14466	CG2	ILE	D	133	-57.558	-21.216	-5.950	1.00	16.11
14470	C	ILE	D	133	-59.810	-22.465	-4.523	1.00	13.46
14471	O	ILE	D	133	-59.000	-22.986	-3.766	1.00	12.91
14472	N	HIS	D	134	-60.864	-21.778	-4.079	1.00	12.05
14474	CA	HIS	D	134	-61.076	-21.591	-2.655	1.00	11.92
14476	CB	HIS	D	134	-62.356	-20.798	-2.399	1.00	11.73
14479	CG	HIS	D	134	-62.709	-20.713	-0.950	1.00	13.46
14480	ND1	HIS	D	134	-62.159	-19.770	-0.110	1.00	16.73
14482	CE1	HIS	D	134	-62.625	-19.951	1.114	1.00	17.63
14484	NE2	HIS	D	134	-63.443	-20.989	1.100	1.00	17.98
14486	CD2	HIS	D	134	-63.508	-21.487	-0.178	1.00	15.83
14488	C	HIS	D	134	-61.138	-22.922	-1.906	1.00	11.24
14489	O	HIS	D	134	-60.493	-23.069	-0.866	1.00	11.16
14490	N	HIS	D	135	-61.915	-23.875	-2.424	1.00	11.13
14492	CA	HIS	D	135	-62.063	-25.177	-1.788	1.00	11.77
14494	CB	HIS	D	135	-63.232	-25.962	-2.386	1.00	12.17
14497	CG	HIS	D	135	-63.548	-27.227	-1.650	1.00	14.36
14498	ND1	HIS	D	135	-63.432	-28.475	-2.226	1.00	17.69
14500	CE1	HIS	D	135	-63.770	-29.398	-1.342	1.00	17.74
14502	NE2	HIS	D	135	-64.119	-28.794	-0.222	1.00	18.87
14504	CD2	HIS	D	135	-63.978	-27.438	-0.384	1.00	15.74
14506	C	HIS	D	135	-60.785	-25.994	-1.877	1.00	11.52
14507	O	HIS	D	135	-60.466	-26.742	-0.973	1.00	12.21
14508	N	VAL	D	136	-60.047	-25.834	-2.963	1.00	10.87
14510	CA	VAL	D	136	-58.761	-26.508	-3.082	1.00	11.39
14512	CB	VAL	D	136	-58.146	-26.343	-4.484	1.00	11.11
14514	CG1	VAL	D	136	-56.743	-26.964	-4.533	1.00	12.59
14518	CG2	VAL	D	136	-59.027	-26.986	-5.514	1.00	12.43

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
14522	C	VAL	D	136	-57.800	-25.993	-2.005	1.00	10.84
14523	O	VAL	D	136	-57.164	-26.775	-1.322	1.00	11.31
14524	N	ARG	D	137	-57.687	-24.681	-1.861	1.00	11.94
14526	CA	ARG	D	137	-56.805	-24.093	-0.861	1.00	12.68
14528	CB	ARG	D	137	-56.778	-22.571	-1.001	1.00	14.51
14531	CG	ARG	D	137	-55.595	-21.923	-0.299	1.00	19.89
14534	CD	ARG	D	137	-54.897	-20.847	-1.152	1.00	26.76
14537	NE	ARG	D	137	-55.390	-19.501	-0.894	1.00	31.90
14539	CZ	ARG	D	137	-54.983	-18.406	-1.543	1.00	35.19
14540	NH1	ARG	D	137	-54.067	-18.482	-2.510	1.00	36.43
14543	NH2	ARG	D	137	-55.495	-17.219	-1.221	1.00	36.67
14546	C	ARG	D	137	-57.230	-24.468	0.553	1.00	12.51
14547	O	ARG	D	137	-56.404	-24.823	1.382	1.00	12.39
14548	N	LYS	D	138	-58.527	-24.378	0.826	1.00	11.73
14550	CA	LYS	D	138	-59.050	-24.673	2.161	1.00	11.89
14552	CB	LYS	D	138	-60.551	-24.404	2.210	1.00	12.56
14555	CG	LYS	D	138	-61.172	-24.562	3.598	1.00	13.69
14558	CD	LYS	D	138	-60.710	-23.506	4.557	1.00	16.65
14561	CE	LYS	D	138	-61.166	-22.106	4.134	1.00	17.59
14564	NZ	LYS	D	138	-60.637	-21.055	5.055	1.00	19.86
14568	C	LYS	D	138	-58.794	-26.133	2.528	1.00	12.02
14569	O	LYS	D	138	-58.415	-26.451	3.642	1.00	11.85
14570	N	SER	D	139	-59.032	-27.014	1.573	1.00	12.18
14572	CA	SER	D	139	-58.779	-28.431	1.766	1.00	12.82
14574	CB	SER	D	139	-59.211	-29.240	0.545	1.00	12.88
14577	OG	SER	D	139	-60.607	-29.149	0.348	1.00	14.15
14579	C	SER	D	139	-57.309	-28.668	2.041	1.00	12.97
14580	O	SER	D	139	-56.964	-29.413	2.941	1.00	13.18
14581	N	MET	D	140	-56.430	-28.040	1.272	1.00	12.95
14583	CA	MET	D	140	-55.005	-28.233	1.501	1.00	13.42
14585	CB	BMET	D	140	-54.178	-27.614	0.373	0.35	13.09
14586	CB	AMET	D	140	-54.176	-27.579	0.394	0.65	14.08
14591	CG	BMET	D	140	-52.804	-28.257	0.194	0.35	12.23
14592	CG	AMET	D	140	-54.253	-28.253	-0.975	0.65	16.83
14597	SD	BMET	D	140	-52.797	-30.072	0.251	0.35	11.20
14598	SD	AMET	D	140	-53.977	-30.062	-1.092	0.65	22.19
14599	CE	BMET	D	140	-53.121	-30.508	-1.461	0.35	10.51
14600	CE	AMET	D	140	-52.538	-30.219	-0.091	0.65	21.51
14607	C	MET	D	140	-54.579	-27.685	2.861	1.00	13.69
14608	O	MET	D	140	-53.776	-28.312	3.545	1.00	13.29
14609	N	GLU	D	141	-55.139	-26.552	3.279	1.00	13.57
14611	CA	GLU	D	141	-54.766	-25.960	4.560	1.00	14.12
14613	CB	GLU	D	141	-55.242	-24.507	4.646	1.00	14.92
14616	CG	BGLU	D	141	-54.515	-23.549	3.717	0.35	15.67
14617	CG	AGLU	D	141	-54.423	-23.592	3.748	0.65	17.47
14622	CD	BGLU	D	141	-53.184	-23.057	4.261	0.35	16.71
14623	CD	AGLU	D	141	-54.927	-22.160	3.668	0.65	21.12
14624	OE1BGLU	D	141		-52.340	-22.635	3.444	0.35	18.75
14625	OE1AGLU	D	141		-54.459	-21.421	2.776	0.65	23.73

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
14626	OE2BGLU	D	141		-52.978	-23.075	5.490	0.35	18.62
14627	OE2AGLU	D	141		-55.769	-21.758	4.493	0.65	25.03
14628	C	GLU	D	141	-55.282	-26.772	5.756	1.00	13.38
14629	O	GLU	D	141	-54.513	-27.074	6.665	1.00	13.18
14630	N	VAL	D	142	-56.559	-27.152	5.737	1.00	12.61
14632	CA	VAL	D	142	-57.178	-27.815	6.886	1.00	12.28
14634	CB	VAL	D	142	-58.718	-27.650	6.888	1.00	12.73
14636	CG1	VAL	D	142	-59.365	-28.445	8.034	1.00	12.36
14640	CG2	VAL	D	142	-59.102	-26.161	6.970	1.00	12.37
14644	C	VAL	D	142	-56.812	-29.297	6.913	1.00	12.15
14645	O	VAL	D	142	-56.454	-29.843	7.954	1.00	12.83
14646	N	ASN	D	143	-56.888	-29.939	5.761	1.00	11.80
14648	CA	ASN	D	143	-56.740	-31.395	5.692	1.00	11.43
14650	CB	ASN	D	143	-57.402	-31.968	4.438	1.00	11.41
14653	CG	ASN	D	143	-58.886	-31.688	4.340	1.00	11.88
14654	OD1	ASN	D	143	-59.516	-31.081	5.236	1.00	12.63
14655	ND2	ASN	D	143	-59.466	-32.119	3.224	1.00	12.05
14658	C	ASN	D	143	-55.286	-31.855	5.675	1.00	11.74
14659	O	ASN	D	143	-55.009	-33.004	6.023	1.00	12.00
14660	N	PHE	D	144	-54.383	-30.986	5.222	1.00	11.59
14662	CA	PHE	D	144	-52.983	-31.344	5.071	1.00	11.27
14664	CB	PHE	D	144	-52.576	-31.334	3.594	1.00	11.63
14667	CG	PHE	D	144	-51.108	-31.476	3.397	1.00	11.99
14668	CD1	PHE	D	144	-50.495	-32.682	3.661	1.00	13.53
14670	CE1	PHE	D	144	-49.126	-32.821	3.531	1.00	12.93
14672	CZ	PHE	D	144	-48.352	-31.753	3.152	1.00	12.87
14674	CE2	PHE	D	144	-48.940	-30.539	2.899	1.00	13.28
14676	CD2	PHE	D	144	-50.316	-30.393	3.019	1.00	12.28
14678	C	PHE	D	144	-52.031	-30.462	5.880	1.00	11.43
14679	O	PHE	D	144	-51.303	-30.963	6.736	1.00	11.53
14680	N	LEU	D	145	-52.005	-29.157	5.623	1.00	11.25
14682	CA	LEU	D	145	-50.991	-28.333	6.275	1.00	11.21
14684	CB	BLEU	D	145	-50.999	-26.903	5.729	0.35	11.15
14685	CB	ALEU	D	145	-50.996	-26.902	5.743	0.65	11.75
14690	CG	BLEU	D	145	-50.576	-26.764	4.264	0.35	10.83
14691	CG	ALEU	D	145	-49.767	-26.083	6.136	0.65	13.29
14694	CD1BLEU	D	145		-50.851	-25.344	3.785	0.35	10.69
14695	CD1ALEU	D	145		-48.498	-26.603	5.467	0.65	15.75
14702	CD2BLEU	D	145		-49.109	-27.119	4.073	0.35	10.66
14703	CD2ALEU	D	145		-50.019	-24.641	5.782	0.65	15.29
14710	C	LEU	D	145	-51.153	-28.334	7.790	1.00	11.17
14711	O	LEU	D	145	-50.167	-28.365	8.517	1.00	11.40
14712	N	SER	D	146	-52.384	-28.321	8.278	1.00	11.31
14714	CA	SER	D	146	-52.560	-28.329	9.725	1.00	11.42
14716	CB	SER	D	146	-54.007	-28.083	10.145	1.00	11.66
14719	OG	SER	D	146	-54.833	-29.186	9.878	1.00	13.09
14721	C	SER	D	146	-52.037	-29.620	10.341	1.00	11.77
14722	O	SER	D	146	-51.561	-29.607	11.465	1.00	12.25
14723	N	TYR	D	147	-52.145	-30.734	9.619	1.00	11.12

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
14725	CA	TYR	D	147	-51.605	-31.999	10.120	1.00	11.42
14727	CB	TYR	D	147	-51.934	-33.161	9.171	1.00	11.36
14730	CG	TYR	D	147	-53.346	-33.717	9.210	1.00	11.23
14731	CD1	TYR	D	147	-54.467	-32.916	9.428	1.00	12.11
14733	CE1	TYR	D	147	-55.750	-33.467	9.442	1.00	12.95
14735	CZ	TYR	D	147	-55.914	-34.820	9.255	1.00	11.31
14736	OH	TYR	D	147	-57.172	-35.367	9.264	1.00	14.08
14738	CE2	TYR	D	147	-54.822	-35.622	9.034	1.00	11.75
14740	CD2	TYR	D	147	-53.561	-35.077	9.021	1.00	11.32
14742	C	TYR	D	147	-50.092	-31.901	10.282	1.00	11.59
14743	O	TYR	D	147	-49.517	-32.438	11.224	1.00	11.00
14744	N	VAL	D	148	-49.433	-31.237	9.340	1.00	11.58
14746	CA	VAL	D	148	-47.996	-31.041	9.432	1.00	11.67
14748	CB	VAL	D	148	-47.421	-30.453	8.116	1.00	11.23
14750	CG1	VAL	D	148	-47.693	-31.404	6.918	1.00	11.97
14754	CG2	VAL	D	148	-45.942	-30.180	8.265	1.00	13.32
14758	C	VAL	D	148	-47.641	-30.136	10.631	1.00	11.45
14759	O	VAL	D	148	-46.741	-30.445	11.396	1.00	11.78
14760	N	VAL	D	149	-48.367	-29.037	10.803	1.00	11.62
14762	CA	VAL	D	149	-48.122	-28.125	11.922	1.00	11.88
14764	CB	VAL	D	149	-49.049	-26.899	11.832	1.00	12.32
14766	CG1	VAL	D	149	-48.972	-26.064	13.104	1.00	13.47
14770	CG2	VAL	D	149	-48.702	-26.076	10.602	1.00	12.52
14774	C	VAL	D	149	-48.310	-28.852	13.255	1.00	12.06
14775	O	VAL	D	149	-47.508	-28.696	14.179	1.00	12.19
14776	N	LEU	D	150	-49.375	-29.636	13.357	1.00	11.92
14778	CA	LEU	D	150	-49.659	-30.389	14.565	1.00	12.22
14780	CB	LEU	D	150	-51.017	-31.092	14.465	1.00	11.92
14783	CG	LEU	D	150	-52.250	-30.193	14.413	1.00	12.25
14785	CD1	LEU	D	150	-53.422	-30.951	13.851	1.00	12.10
14789	CD2	LEU	D	150	-52.601	-29.653	15.798	1.00	12.57
14793	C	LEU	D	150	-48.554	-31.400	14.860	1.00	12.62
14794	O	LEU	D	150	-48.148	-31.564	16.010	1.00	12.61
14795	N	THR	D	151	-48.044	-32.049	13.815	1.00	12.12
14797	CA	THR	D	151	-46.965	-33.012	13.962	1.00	12.39
14799	CB	THR	D	151	-46.731	-33.732	12.634	1.00	12.40
14801	OG1	THR	D	151	-47.882	-34.531	12.340	1.00	12.42
14803	CG2	THR	D	151	-45.587	-34.700	12.744	1.00	14.70
14807	C	THR	D	151	-45.672	-32.352	14.434	1.00	12.44
14808	O	THR	D	151	-45.022	-32.846	15.342	1.00	13.11
14809	N	VAL	D	152	-45.300	-31.231	13.824	1.00	12.26
14811	CA	VAL	D	152	-44.112	-30.502	14.251	1.00	12.40
14813	CB	VAL	D	152	-43.878	-29.235	13.390	1.00	12.69
14815	CG1	VAL	D	152	-42.830	-28.346	14.012	1.00	12.13
14819	CG2	VAL	D	152	-43.461	-29.616	11.977	1.00	13.01
14823	C	VAL	D	152	-44.213	-30.123	15.735	1.00	12.74
14824	O	VAL	D	152	-43.237	-30.237	16.491	1.00	13.27
14825	N	ALA	D	153	-45.397	-29.700	16.156	1.00	12.87
14827	CA	ALA	D	153	-45.599	-29.267	17.536	1.00	13.52



# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
14829	CB	ALA	D	153	-46.922	-28.571	17.670	1.00	13.63
14833	C	ALA	D	153	-45.540	-30.437	18.512	1.00	13.79
14834	O	ALA	D	153	-45.119	-30.272	19.665	1.00	14.50
14835	N	ALA	D	154	-45.971	-31.604	18.046	1.00	13.25
14837	CA	ALA	D	154	-46.109	-32.789	18.893	1.00	13.82
14839	CB	ALA	D	154	-47.241	-33.672	18.376	1.00	13.63
14843	C	ALA	D	154	-44.830	-33.604	18.961	1.00	13.85
14844	O	ALA	D	154	-44.684	-34.414	19.873	1.00	14.35
14845	N	LEU	D	155	-43.916	-33.414	18.012	1.00	14.42
14847	CA	LEU	D	155	-42.821	-34.371	17.849	1.00	15.07
14849	CB	LEU	D	155	-42.026	-34.139	16.552	1.00	15.84
14852	CG	LEU	D	155	-41.075	-35.282	16.161	1.00	17.72
14854	CD1	LEU	D	155	-40.261	-34.887	14.935	1.00	18.37
14858	CD2	LEU	D	155	-41.819	-36.602	15.919	1.00	18.95
14862	C	LEU	D	155	-41.894	-34.453	19.071	1.00	15.23
14863	O	LEU	D	155	-41.534	-35.562	19.456	1.00	14.88
14864	N	PRO	D	156	-41.490	-33.334	19.678	1.00	15.44
14865	CA	PRO	D	156	-40.676	-33.428	20.900	1.00	15.55
14867	CB	PRO	D	156	-40.567	-31.972	21.371	1.00	15.65
14870	CG	PRO	D	156	-40.668	-31.176	20.096	1.00	15.98
14873	CD	PRO	D	156	-41.679	-31.931	19.257	1.00	15.13
14876	C	PRO	D	156	-41.295	-34.350	21.957	1.00	15.37
14877	O	PRO	D	156	-40.581	-35.199	22.491	1.00	15.67
14878	N	MET	D	157	-42.593	-34.227	22.215	1.00	15.49
14880	CA	MET	D	157	-43.256	-35.056	23.224	1.00	15.30
14882	CB	MET	D	157	-44.658	-34.524	23.552	1.00	15.69
14885	CG	MET	D	157	-44.654	-33.294	24.462	1.00	15.80
14888	SD	MET	D	157	-46.309	-32.760	24.840	1.00	17.1
14889	CE	MET	D	157	-46.889	-32.166	23.246	1.00	17.42
14893	C	MET	D	157	-43.349	-36.510	22.779	1.00	15.21
14894	O	MET	D	157	-43.202	-37.424	23.584	1.00	15.64
14895	N	LEU	D	158	-43.596	-36.727	21.490	1.00	15.26
14897	CA	LEU	D	158	-43.698	-38.082	20.969	1.00	15.21
14899	CB	LEU	D	158	-44.272	-38.063	19.549	1.00	15.06
14902	CG	LEU	D	158	-45.734	-37.624	19.437	1.00	15.21
14904	CD1	LEU	D	158	-46.109	-37.427	17.974	1.00	15.55
14908	CD2	LEU	D	158	-46.667	-38.615	20.107	1.00	15.84
14912	C	LEU	D	158	-42.341	-38.792	20.990	1.00	15.75
14913	O	LEU	D	158	-42.278	-39.986	21.216	1.00	15.57
14914	N	LYS	D	159	-41.261	-38.053	20.767	1.00	16.68
14916	CA	LYS	D	159	-39.918	-38.621	20.838	1.00	17.77
14918	CB	LYS	D	159	-38.872	-37.625	20.337	1.00	18.05
14921	CG	LYS	D	159	-38.860	-37.462	18.820	1.00	19.21
14924	CD	LYS	D	159	-37.937	-36.337	18.379	1.00	21.12
14927	CE	LYS	D	159	-37.630	-36.418	16.890	1.00	22.31
14930	NZ	LYS	D	159	-37.033	-35.145	16.377	1.00	24.14
14934	C	LYS	D	159	-39.609	-39.039	22.272	1.00	18.27
14935	O	LYS	D	159	-38.996	-40.074	22.499	1.00	18.31
14936	N	GLN	D	160	-40.062	-38.237	23.233	1.00	18.71

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
14938	CA	GLN	D	160	-39.853	-38.535	24.651	1.00	19.46
14940	CB	GLN	D	160	-40.383	-37.380	25.510	1.00	20.06
14943	CG	GLN	D	160	-39.992	-37.443	26.978	1.00	23.30
14946	CD	GLN	D	160	-38.724	-36.661	27.278	1.00	26.68
14947	OE1	GLN	D	160	-37.635	-37.231	27.304	1.00	30.11
14948	NE2	GLN	D	160	-38.863	-35.354	27.503	1.00	29.35
14951	C	GLN	D	160	-40.549	-39.838	25.057	1.00	19.08
14952	O	GLN	D	160	-40.020	-40.606	25.866	1.00	19.23
14953	N	SER	D	161	-41.726	-40.084	24.483	1.00	18.48
14955	CA	SER	D	161	-42.544	-41.244	24.825	1.00	17.81
14957	CB	SER	D	161	-44.017	-40.838	24.883	1.00	18.04
14960	OG	SER	D	161	-44.522	-40.539	23.590	1.00	17.79
14962	C	SER	D	161	-42.406	-42.434	23.868	1.00	17.46
14963	O	SER	D	161	-43.040	-43.469	24.089	1.00	17.17
14964	N	ASN	D	162	-41.596	-42.289	22.817	1.00	17.13
14966	CA	ASN	D	162	-41.529	-43.282	21.739	1.00	17.07
14968	CB	ASN	D	162	-40.880	-44.595	22.218	1.00	17.45
14971	CG	ASN	D	162	-39.460	-44.406	22.719	1.00	19.25
14972	OD1	ASN	D	162	-38.670	-43.688	22.121	1.00	22.06
14973	ND2	ASN	D	162	-39.129	-45.070	23.819	1.00	22.61
14976	C	ASN	D	162	-42.934	-43.554	21.206	1.00	16.48
14977	O	ASN	D	162	-43.358	-44.702	21.069	1.00	16.42
14978	N	GLY	D	163	-43.656	-42.476	20.917	1.00	15.72
14980	CA	GLY	D	163	-45.074	-42.545	20.654	1.00	15.15
14983	C	GLY	D	163	-45.428	-42.747	19.196	1.00	15.00
14984	O	GLY	D	163	-44.643	-43.276	18.424	1.00	14.53
14985	N	SER	D	164	-46.617	-42.289	18.829	1.00	14.75
14987	CA	SER	D	164	-47.241	-42.667	17.569	1.00	14.91
14989	CB	SER	D	164	-48.157	-43.866	17.786	1.00	15.31
14992	OG	SER	D	164	-47.453	-44.968	18.339	1.00	16.88
14994	C	SER	D	164	-48.060	-41.527	16.983	1.00	14.53
14995	O	SER	D	164	-48.734	-40.802	17.704	1.00	14.25
14996	N	ILE	D	165	-48.002	-41.406	15.666	1.00	13.80
14998	CA	ILE	D	165	-48.855	-40.514	14.888	1.00	13.66
15000	CB	ILE	D	165	-48.006	-39.615	13.959	1.00	14.14
15002	CG1	ILE	D	165	-47.013	-38.794	14.776	1.00	15.11
15005	CD1	ILE	D	165	-45.904	-38.192	13.957	1.00	16.22
15009	CG2	ILE	D	165	-48.917	-38.686	13.134	1.00	15.00
15013	C	ILE	D	165	-49.796	-41.375	14.053	1.00	13.20
15014	O	ILE	D	165	-49.364	-42.303	13.377	1.00	14.27
15015	N	VAL	D	166	-51.080	-41.061	14.104	1.00	13.09
15017	CA	VAL	D	166	-52.097	-41.756	13.339	1.00	13.33
15019	CB	VAL	D	166	-53.141	-42.417	14.267	1.00	13.57
15021	CG1	VAL	D	166	-54.227	-43.086	13.465	1.00	14.05
15025	CG2	VAL	D	166	-52.461	-43.384	15.233	1.00	15.39
15029	C	VAL	D	166	-52.759	-40.741	12.416	1.00	13.23
15030	O	VAL	D	166	-53.308	-39.742	12.878	1.00	13.96
15031	N	VAL	D	167	-52.671	-40.980	11.109	1.00	12.50
15033	CA	VAL	D	167	-53.198	-40.073	10.097	1.00	12.31

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
15035	CB	VAL	D	167	-52.099	-39.737	9.050	1.00	12.49
15037	CG1	VAL	D	167	-52.641	-38.854	7.945	1.00	13.35
15041	CG2	VAL	D	167	-50.898	-39.081	9.740	1.00	13.19
15045	C	VAL	D	167	-54.387	-40.747	9.419	1.00	12.53
15046	O	VAL	D	167	-54.239	-41.804	8.824	1.00	12.75
15047	N	VAL	D	168	-55.577	-40.152	9.530	1.00	12.48
15049	CA	VAL	D	168	-56.761	-40.753	8.938	1.00	12.98
15051	CB	VAL	D	168	-58.031	-40.456	9.741	1.00	13.08
15053	CG1	VAL	D	168	-59.240	-41.168	9.111	1.00	14.02
15057	CG2	VAL	D	168	-57.837	-40.895	11.190	1.00	14.06
15061	C	VAL	D	168	-56.913	-40.294	7.498	1.00	13.46
15062	O	VAL	D	168	-56.934	-39.104	7.211	1.00	13.66
15063	N	SER	D	169	-57.010	-41.268	6.607	1.00	13.29
15065	CA	SER	D	169	-57.144	-41.029	5.176	1.00	13.25
15067	CB	SER	D	169	-55.804	-41.227	4.462	1.00	13.35
15070	OG	SER	D	169	-55.870	-40.734	3.132	1.00	13.38
15072	C	SER	D	169	-58.246	-41.928	4.615	1.00	13.56
15073	O	SER	D	169	-59.124	-42.353	5.338	1.00	14.40
15074	N	SER	D	170	-58.159	-42.260	3.341	1.00	13.20
15076	CA	SER	D	170	-59.340	-42.510	2.542	1.00	12.90
15078	CB	SER	D	170	-59.874	-41.159	2.052	1.00	13.48
15081	OG	SER	D	170	-59.887	-40.186	3.099	1.00	15.10
15083	C	SER	D	170	-59.007	-43.334	1.321	1.00	12.68
15084	O	SER	D	170	-57.889	-43.254	0.811	1.00	12.07
15085	N	LEU	D	171	-59.976	-44.101	0.828	1.00	12.19
15087	CA	LEU	D	171	-59.827	-44.707	-0.494	1.00	11.65
15089	CB	LEU	D	171	-61.105	-45.428	-0.944	1.00	12.24
15092	CG	LEU	D	171	-61.486	-46.674	-0.132	1.00	12.74
15094	CD1	LEU	D	171	-60.434	-47.775	-0.252	1.00	14.53
15098	CD2	LEU	D	171	-62.845	-47.202	-0.546	1.00	13.94
15102	C	LEU	D	171	-59.445	-43.653	-1.524	1.00	12.15
15103	O	LEU	D	171	-58.603	-43.903	-2.375	1.00	11.57
15104	N	ALA	D	172	-60.058	-42.472	-1.447	1.00	12.42
15106	CA	ALA	D	172	-59.747	-41.384	-2.377	1.00	12.48
15108	CB	ALA	D	172	-60.864	-40.351	-2.370	1.00	13.25
15112	C	ALA	D	172	-58.384	-40.711	-2.114	1.00	12.58
15113	O	ALA	D	172	-57.998	-39.780	-2.834	1.00	12.96
15114	N	GLY	D	173	-57.659	-41.200	-1.111	1.00	11.85
15116	CA	GLY	D	173	-56.257	-40.886	-0.895	1.00	11.70
15119	C	GLY	D	173	-55.257	-41.920	-1.429	1.00	11.80
15120	O	GLY	D	173	-54.046	-41.758	-1.212	1.00	11.88
15121	N	LYS	D	174	-55.758	-42.963	-2.096	1.00	12.00
15123	CA	LYS	D	174	-54.931	-44.027	-2.691	1.00	11.97
15125	CB	LYS	D	174	-55.116	-45.339	-1.920	1.00	12.05
15128	CG	LYS	D	174	-54.496	-45.343	-0.548	1.00	11.63
15131	CD	LYS	D	174	-52.975	-45.199	-0.600	1.00	11.12
15134	CE	LYS	D	174	-52.325	-45.517	0.717	1.00	12.30
15137	NZ	LYS	D	174	-50.833	-45.584	0.600	1.00	12.07
15141	C	LYS	D	174	-55.239	-44.279	-4.159	1.00	11.80

## FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
15142	O	LYS	D	174	-54.362	-44.704	-4.909	1.00	12.06
15143	N	VAL	D	175	-56.491	-44.050	-4.561	1.00	11.67
15145	CA	VAL	D	175	-56.905	-44.128	-5.960	1.00	11.71
15147	CB	VAL	D	175	-57.622	-45.466	-6.313	1.00	12.10
15149	CG1	VAL	D	175	-58.954	-45.595	-5.606	1.00	12.79
15153	CG2	VAL	D	175	-56.724	-46.645	-5.993	1.00	11.66
15157	C	VAL	D	175	-57.797	-42.926	-6.272	1.00	12.32
15158	O	VAL	D	175	-58.206	-42.196	-5.361	1.00	12.76
15159	N	ALA	D	176	-58.063	-42.730	-7.557	1.00	12.84
15161	CA	ALA	D	176	-58.757	-41.547	-8.055	1.00	13.12
15163	CB	ALA	D	176	-58.150	-41.115	-9.376	1.00	13.63
15167	C	ALA	D	176	-60.252	-41.773	-8.222	1.00	13.33
15168	O	ALA	D	176	-60.681	-42.764	-8.827	1.00	14.42
15169	N	TYR	D	177	-61.029	-40.810	-7.714	1.00	12.82
15171	CA	TYR	D	177	-62.486	-40.765	-7.851	1.00	12.83
15173	CB	TYR	D	177	-63.194	-40.922	-6.499	1.00	12.82
15176	CG	TYR	D	177	-63.089	-42.274	-5.857	1.00	12.62
15177	CD1	TYR	D	177	-61.981	-42.619	-5.094	1.00	13.75
15179	CE1	TYR	D	177	-61.880	-43.852	-4.483	1.00	12.93
15181	CZ	TYR	D	177	-62.904	-44.766	-4.628	1.00	12.68
15182	OH	TYR	D	177	-62.818	-46.001	-4.033	1.00	13.98
15184	CE2	TYR	D	177	-64.018	-44.449	-5.371	1.00	12.80
15186	CD2	TYR	D	177	-64.112	-43.200	-5.979	1.00	13.06
15188	C	TYR	D	177	-62.890	-39.401	-8.378	1.00	12.76
15189	O	TYR	D	177	-62.291	-38.392	-8.006	1.00	13.31
15190	N	PRO	D	178	-63.945	-39.344	-9.183	1.00	13.20
15191	CA	PRO	D	178	-64.533	-38.054	-9.554	1.00	12.52
15193	CB	PRO	D	178	-65.510	-38.420	-10.662	1.00	12.78
15196	CG	PRO	D	178	-65.894	-39.818	-10.371	1.00	12.91
15199	CD	PRO	D	178	-64.716	-40.471	-9.734	1.00	12.44
15202	C	PRO	D	178	-65.271	-37.484	-8.351	1.00	12.88
15203	O	PRO	D	178	-65.625	-38.232	-7.445	1.00	13.12
15204	N	MET	D	179	-65.480	-36.178	-8.364	1.00	12.98
15206	CA	MET	D	179	-66.344	-35.459	-7.411	1.00	13.64
15208	CB	MET	D	179	-67.675	-36.199	-7.166	1.00	14.25
15211	CG	BMET	D	179	-68.422	-36.571	-8.440	0.35	15.21
15212	CG	AMET	D	179	-68.414	-36.637	-8.425	0.65	16.54
15217	SD	BMET	D	179	-70.166	-36.914	-8.144	0.35	16.87
15218	SD	AMET	D	179	-68.576	-35.360	-9.671	0.65	20.23
15219	CE	BMET	D	179	-70.821	-35.261	-7.929	0.35	16.68
15220	CE	AMET	D	179	-69.117	-36.347	-11.067	0.65	20.59
15227	C	MET	D	179	-65.695	-35.119	-6.075	1.00	13.27
15228	O	MET	D	179	-66.333	-34.495	-5.225	1.00	13.68
15229	N	VAL	D	180	-64.433	-35.502	-5.890	1.00	12.25
15231	CA	VAL	D	180	-63.702	-35.236	-4.653	1.00	12.76
15233	CB	VAL	D	180	-63.665	-36.503	-3.721	1.00	13.10
15235	CG1	VAL	D	180	-65.027	-36.779	-3.125	1.00	14.58
15239	CG2	VAL	D	180	-63.159	-37.720	-4.466	1.00	14.10
15243	C	VAL	D	180	-62.276	-34.741	-4.944	1.00	12.06

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
15244	O	VAL	D	180	-61.352	-35.110	-4.247	1.00	12.07
15245	N	ALA	D	181	-62.087	-33.917	-5.974	1.00	12.35
15247	CA	ALA	D	181	-60.731	-33.571	-6.418	1.00	11.75
15249	CB	ALA	D	181	-60.780	-32.761	-7.692	1.00	11.91
15253	C	ALA	D	181	-59.872	-32.852	-5.372	1.00	11.81
15254	O	ALA	D	181	-58.743	-33.250	-5.115	1.00	11.83
15255	N	ALA	D	182	-60.403	-31.780	-4.802	1.00	11.56
15257	CA	ALA	D	182	-59.710	-31.026	-3.757	1.00	11.76
15259	CB	ALA	D	182	-60.550	-29.856	-3.319	1.00	12.24
15263	C	ALA	D	182	-59.371	-31.907	-2.560	1.00	11.43
15264	O	ALA	D	182	-58.273	-31.868	-2.026	1.00	11.78
15265	N	TYR	D	183	-60.344	-32.691	-2.124	1.00	11.14
15267	CA	TYR	D	183	-60.155	-33.604	-1.015	1.00	10.76
15269	CB	TYR	D	183	-61.472	-34.303	-0.742	1.00	11.17
15272	CG	TYR	D	183	-61.456	-35.413	0.262	1.00	10.91
15273	CD1	TYR	D	183	-61.651	-35.156	1.618	1.00	11.30
15275	CE1	TYR	D	183	-61.685	-36.187	2.533	1.00	13.47
15277	CZ	TYR	D	183	-61.538	-37.486	2.095	1.00	11.68
15278	OH	TYR	D	183	-61.603	-38.527	2.982	1.00	13.57
15280	CE2	TYR	D	183	-61.335	-37.765	0.762	1.00	11.29
15282	CD2	TYR	D	183	-61.313	-36.741	-0.145	1.00	11.77
15284	C	TYR	D	183	-59.094	-34.637	-1.316	1.00	10.53
15285	O	TYR	D	183	-58.204	-34.874	-0.506	1.00	10.70
15286	N	SER	D	184	-59.182	-35.237	-2.504	1.00	10.89
15288	CA	SER	D	184	-58.221	-36.253	-2.906	1.00	10.79
15290	CB	BSER	D	184	-58.603	-36.848	-4.262	0.35	11.04
15291	CB	ASER	D	184	-58.565	-36.823	-4.280	0.65	11.45
15296	OG	BSER	D	184	-57.682	-37.848	-4.660	0.35	11.04
15297	OG	ASER	D	184	-59.818	-37.464	-4.283	0.65	13.47
15300	C	SER	D	184	-56.811	-35.681	-2.947	1.00	10.83
15301	O	SER	D	184	-55.870	-36.331	-2.496	1.00	11.04
15302	N	ALA	D	185	-56.660	-34.469	-3.470	1.00	10.73
15304	CA	ALA	D	185	-55.349	-33.825	-3.483	1.00	10.61
15306	CB	ALA	D	185	-55.444	-32.431	-4.079	1.00	10.45
15310	C	ALA	D	185	-54.763	-33.779	-2.068	1.00	10.48
15311	O	ALA	D	185	-53.597	-34.105	-1.860	1.00	10.31
15312	N	SER	D	186	-55.575	-33.388	-1.090	1.00	10.14
15314	CA	SER	D	186	-55.101	-33.252	0.273	1.00	10.60
15316	CB	SER	D	186	-56.096	-32.459	1.129	1.00	11.18
15319	OG	SER	D	186	-57.263	-33.205	1.408	1.00	10.48
15321	C	SER	D	186	-54.758	-34.592	0.903	1.00	10.50
15322	O	SER	D	186	-53.777	-34.695	1.634	1.00	10.89
15323	N	LYS	D	187	-55.532	-35.634	0.597	1.00	10.33
15325	CA	LYS	D	187	-55.266	-36.947	1.165	1.00	10.70
15327	CB	LYS	D	187	-56.499	-37.835	1.083	1.00	10.66
15330	CG	LYS	D	187	-57.680	-37.332	1.906	1.00	11.81
15333	CD	LYS	D	187	-57.366	-37.252	3.401	1.00	11.48
15336	CE	LYS	D	187	-58.624	-37.167	4.229	1.00	13.25
15339	NZ	LYS	D	187	-58.384	-37.209	5.713	1.00	12.84

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
15343	C	LYS	D	187	-54.060	-37.612	0.504	1.00	9.93
15344	O	LYS	D	187	-53.281	-38.260	1.178	1.00	10.69
15345	N	PHE	D	188	-53.913	-37.471	-0.818	1.00	10.29
15347	CA	PHE	D	188	-52.691	-37.909	-1.486	1.00	10.03
15349	CB	PHE	D	188	-52.760	-37.636	-2.993	1.00	9.75
15352	CG	PHE	D	188	-53.339	-38.773	-3.815	1.00	9.38
15353	CD1	PHE	D	188	-52.537	-39.475	-4.719	1.00	9.40
15355	CE1	PHE	D	188	-53.070	-40.505	-5.505	1.00	9.92
15357	CZ	PHE	D	188	-54.410	-40.836	-5.391	1.00	9.54
15359	CE2	PHE	D	188	-55.215	-40.139	-4.519	1.00	10.24
15361	CD2	PHE	D	188	-54.685	-39.104	-3.740	1.00	9.53
15363	C	PHE	D	188	-51.475	-37.211	-0.874	1.00	9.72
15364	O	PHE	D	188	-50.461	-37.847	-0.596	1.00	9.85
15365	N	ALA	D	189	-51.591	-35.910	-0.610	1.00	10.02
15367	CA	ALA	D	189	-50.498	-35.141	-0.028	1.00	10.22
15369	CB	ALA	D	189	-50.905	-33.683	0.145	1.00	10.50
15373	C	ALA	D	189	-50.070	-35.732	1.315	1.00	10.27
15374	O	ALA	D	189	-48.884	-35.826	1.607	1.00	10.33
15375	N	LEU	D	190	-51.037	-36.128	2.137	1.00	10.50
15377	CA	LEU	D	190	-50.728	-36.764	3.413	1.00	10.66
15379	CB	LEU	D	190	-52.008	-37.123	4.177	1.00	10.95
15382	CG	LEU	D	190	-52.829	-35.979	4.787	1.00	11.91
15384	CD1	LEU	D	190	-54.142	-36.518	5.332	1.00	12.38
15388	CD2	LEU	D	190	-52.091	-35.246	5.912	1.00	11.46
15392	C	LEU	D	190	-49.888	-38.013	3.233	1.00	10.40
15393	O	LEU	D	190	-48.952	-38.244	3.988	1.00	11.16
15394	N	ASP	D	191	-50.261	-38.840	2.273	1.00	10.44
15396	CA	ASP	D	191	-49.523	-40.074	2.022	1.00	10.73
15398	CB	ASP	D	191	-50.226	-40.870	0.925	1.00	10.64
15401	CG	ASP	D	191	-49.665	-42.255	0.725	1.00	11.50
15402	OD1	ASP	D	191	-48.766	-42.711	1.474	1.00	13.36
15403	OD2	ASP	D	191	-50.100	-42.963	-0.199	1.00	11.51
15404	C	ASP	D	191	-48.089	-39.739	1.638	1.00	10.97
15405	O	ASP	D	191	-47.156	-40.267	2.209	1.00	11.07
15406	N	GLY	D	192	-47.902	-38.859	0.658	1.00	11.14
15408	CA	GLY	D	192	-46.571	-38.476	0.262	1.00	10.94
15411	C	GLY	D	192	-45.744	-37.935	1.417	1.00	10.89
15412	O	GLY	D	192	-44.600	-38.341	1.630	1.00	11.73
15413	N	PHE	D	193	-46.310	-37.005	2.170	1.00	10.77
15415	CA	PHE	D	193	-45.563	-36.376	3.239	1.00	10.41
15417	CB	PHE	D	193	-46.321	-35.197	3.841	1.00	10.56
15420	CG	PHE	D	193	-45.517	-34.458	4.860	1.00	10.85
15421	CD1	PHE	D	193	-45.712	-34.683	6.218	1.00	12.95
15423	CE1	PHE	D	193	-44.936	-34.008	7.156	1.00	13.81
15425	CZ	PHE	D	193	-43.960	-33.145	6.732	1.00	12.26
15427	CE2	PHE	D	193	-43.760	-32.925	5.388	1.00	12.93
15429	CD2	PHE	D	193	-44.523	-33.586	4.466	1.00	11.71
15431	C	PHE	D	193	-45.223	-37.372	4.350	1.00	10.87
15432	O	PHE	D	193	-44.065	-37.537	4.700	1.00	10.74

## FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
15433	N	PHE	D	194	-46.247	-38.010	4.913	1.00	10.76
15435	CA	PHE	D	194	-46.059	-38.857	6.080	1.00	10.89
15437	CB	PHE	D	194	-47.387	-39.114	6.805	1.00	10.83
15440	CG	PHE	D	194	-47.813	-37.944	7.630	1.00	11.64
15441	CD1	PHE	D	194	-48.728	-37.025	7.143	1.00	12.38
15443	CE1	PHE	D	194	-49.079	-35.913	7.901	1.00	13.65
15445	CZ	PHE	D	194	-48.509	-35.715	9.139	1.00	14.05
15447	CE2	PHE	D	194	-47.595	-36.610	9.625	1.00	13.74
15449	CD2	PHE	D	194	-47.240	-37.718	8.881	1.00	12.23
15451	C	PHE	D	194	-45.307	-40.127	5.766	1.00	11.11
15452	O	PHE	D	194	-44.544	-40.591	6.601	1.00	10.96
15453	N	SER	D	195	-45.468	-40.654	4.561	1.00	11.27
15455	CA	SER	D	195	-44.670	-41.818	4.151	1.00	11.16
15457	CB	SER	D	195	-45.227	-42.477	2.891	1.00	11.21
15460	OG	SER	D	195	-46.569	-42.855	3.049	1.00	12.25
15462	C	SER	D	195	-43.195	-41.447	3.968	1.00	11.63
15463	O	SER	D	195	-42.323	-42.259	4.250	1.00	11.72
15464	N	SER	D	196	-42.907	-40.223	3.521	1.00	11.82
15466	CA	SER	D	196	-41.528	-39.743	3.417	1.00	12.68
15468	CB	BSER	D	196	-41.477	-38.473	2.576	0.35	12.82
15469	CB	ASER	D	196	-41.445	-38.438	2.605	0.65	13.01
15474	OG	BSER	D	196	-41.916	-38.768	1.264	0.35	13.11
15475	OG	ASER	D	196	-40.159	-37.832	2.726	0.65	13.50
15478	C	SER	D	196	-40.897	-39.531	4.785	1.00	13.16
15479	O	SER	D	196	-39.767	-39.979	5.006	1.00	13.27
15480	N	ILE	D	197	-41.597	-38.868	5.702	1.00	13.62
15482	CA	ILE	D	197	-41.026	-38.702	7.035	1.00	14.41
15484	CB	ILE	D	197	-41.724	-37.612	7.915	1.00	15.51
15486	CG1	ILE	D	197	-43.181	-37.899	8.188	1.00	17.59
15489	CD1	ILE	D	197	-43.676	-37.176	9.448	1.00	19.54
15493	CG2	ILE	D	197	-41.548	-36.202	7.321	1.00	16.11
15497	C	ILE	D	197	-40.876	-40.055	7.739	1.00	13.72
15498	O	ILE	D	197	-39.927	-40.245	8.474	1.00	13.97
15499	N	ARG	D	198	-41.753	-41.019	7.465	1.00	13.47
15501	CA	ARG	D	198	-41.574	-42.360	8.024	1.00	13.78
15503	CB	ARG	D	198	-42.695	-43.322	7.605	1.00	13.72
15506	CG	ARG	D	198	-42.692	-44.612	8.410	1.00	14.65
15509	CD	ARG	D	198	-43.605	-45.688	7.880	1.00	14.61
15512	NE	ARG	D	198	-45.018	-45.394	8.055	1.00	14.15
15514	CZ	ARG	D	198	-45.892	-45.135	7.080	1.00	14.55
15515	NH1	ARG	D	198	-45.518	-45.074	5.811	1.00	15.58
15518	NH2	ARG	D	198	-47.165	-44.910	7.376	1.00	15.91
15521	C	ARG	D	198	-40.221	-42.926	7.608	1.00	13.72
15522	O	ARG	D	198	-39.519	-43.512	8.436	1.00	14.21
15523	N	LYS	D	199	-39.853	-42.749	6.338	1.00	14.06
15525	CA	LYS	D	199	-38.542	-43.211	5.843	1.00	13.97
15527	CB	LYS	D	199	-38.355	-42.988	4.331	1.00	14.36
15530	CG	LYS	D	199	-39.406	-43.561	3.421	1.00	15.66
15533	CD	LYS	D	199	-39.556	-45.040	3.560	1.00	16.81

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
15536	CE	LYS	D	199	-40.237	-45.645	2.334	1.00	17.11
15539	NZ	LYS	D	199	-40.507	-47.104	2.519	1.00	17.96
15543	C	LYS	D	199	-37.421	-42.481	6.585	1.00	14.43
15544	O	LYS	D	199	-36.432	-43.086	6.988	1.00	14.18
15545	N	GLU	D	200	-37.583	-41.181	6.782	1.00	14.22
15547	CA	GLU	D	200	-36.583	-40.387	7.473	1.00	14.56
15549	CB	GLU	D	200	-36.946	-38.903	7.425	1.00	14.70
15552	CG	GLU	D	200	-36.863	-38.326	6.024	1.00	14.97
15555	CD	GLU	D	200	-37.170	-36.845	5.957	1.00	15.33
15556	OE1	GLU	D	200	-37.285	-36.335	4.820	1.00	15.96
15557	OE2	GLU	D	200	-37.290	-36.202	7.013	1.00	16.35
15558	C	GLU	D	200	-36.404	-40.830	8.920	1.00	15.09
15559	O	GLU	D	200	-35.285	-40.901	9.407	1.00	15.03
15560	N	TYR	D	201	-37.504	-41.139	9.600	1.00	15.56
15562	CA	TYR	D	201	-37.423	-41.563	10.998	1.00	16.19
15564	CB	TYR	D	201	-38.811	-41.626	11.640	1.00	16.26
15567	CG	TYR	D	201	-39.468	-40.279	11.867	1.00	16.71
15568	CD1	TYR	D	201	-38.822	-39.084	11.539	1.00	19.19
15570	CE1	TYR	D	201	-39.432	-37.860	11.744	1.00	20.37
15572	CZ	TYR	D	201	-40.702	-37.807	12.269	1.00	21.02
15573	OH	TYR	D	201	-41.301	-36.579	12.466	1.00	25.67
15575	CE2	TYR	D	201	-41.363	-38.967	12.613	1.00	19.75
15577	CD2	TYR	D	201	-40.741	-40.202	12.414	1.00	19.14
15579	C	TYR	D	201	-36.710	-42.908	11.097	1.00	17.17
15580	O	TYR	D	201	-36.003	-43.164	12.064	1.00	16.78
15581	N	SER	D	202	-36.858	-43.751	10.083	1.00	18.13
15583	CA	SER	D	202	-36.151	-45.035	10.066	1.00	19.55
15585	CB	BSER	D	202	-36.668	-45.926	8.935	0.35	19.40
15586	CB	ASER	D	202	-36.669	-45.928	8.943	0.65	19.66
15591	OG	BSER	D	202	-35.949	-47.146	8.880	0.35	19.12
15592	OG	ASER	D	202	-38.012	-46.291	9.185	0.65	21.86
15595	C	SER	D	202	-34.649	-44.837	9.931	1.00	20.43
15596	O	SER	D	202	-33.878	-45.418	10.691	1.00	20.71
15597	N	VAL	D	203	-34.229	-44.010	8.978	1.00	21.46
15599	CA	VAL	D	203	-32.802	-43.764	8.770	1.00	22.67
15601	CB	VAL	D	203	-32.506	-43.057	7.417	1.00	23.02
15603	CG1	VAL	D	203	-33.081	-43.848	6.255	1.00	24.57
15607	CG2	VAL	D	203	-33.036	-41.650	7.395	1.00	24.24
15611	C	VAL	D	203	-32.167	-42.984	9.929	1.00	22.62
15612	O	VAL	D	203	-30.985	-43.170	10.227	1.00	22.58
15613	N	SER	D	204	-32.951	-42.137	10.593	1.00	22.63
15615	CA	SER	D	204	-32.444	-41.316	11.695	1.00	22.58
15617	CB	BSER	D	204	-33.034	-39.900	11.645	0.35	22.66
15618	CB	ASER	D	204	-33.084	-39.925	11.657	0.65	22.83
15623	OG	BSER	D	204	-34.437	-39.897	11.831	0.35	22.01
15624	OG	ASER	D	204	-32.697	-39.217	10.492	0.65	23.07
15627	C	SER	D	204	-32.697	-41.971	13.058	1.00	22.65
15628	O	SER	D	204	-32.327	-41.415	14.088	1.00	22.96
15629	N	ARG	D	205	-33.317	-43.153	13.050	1.00	22.36



## FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
15631	CA	ARG	D	205	-33.592	-43.926	14.265	1.00	22.65
15633	CB	ARG	D	205	-32.283	-44.423	14.886	1.00	23.12
15636	CG	ARG	D	205	-31.334	-45.058	13.871	1.00	25.75
15639	CD	ARG	D	205	-31.493	-46.563	13.712	1.00	29.10
15642	NE	ARG	D	205	-30.393	-47.291	14.348	1.00	31.47
15644	CZ	ARG	D	205	-29.203	-47.543	13.789	1.00	34.01
15645	NH1	ARG	D	205	-28.917	-47.139	12.550	1.00	35.34
15648	NH2	ARG	D	205	-28.286	-48.212	14.477	1.00	34.53
15651	C	ARG	D	205	-34.436	-43.147	15.281	1.00	21.76
15652	O	ARG	D	205	-34.196	-43.185	16.492	1.00	21.96
15653	N	VAL	D	206	-35.425	-42.427	14.763	1.00	20.35
15655	CA	VAL	D	206	-36.440	-41.778	15.578	1.00	19.41
15657	CB	VAL	D	206	-37.038	-40.562	14.843	1.00	19.52
15659	CG1	VAL	D	206	-38.266	-40.022	15.569	1.00	18.94
15663	CG2	VAL	D	206	-35.986	-39.481	14.663	1.00	20.11
15667	C	VAL	D	206	-37.533	-42.809	15.845	1.00	18.66
15668	O	VAL	D	206	-38.142	-43.318	14.910	1.00	17.53
15669	N	ASN	D	207	-37.789	-43.100	17.118	1.00	17.87
15671	CA	ASN	D	207	-38.707	-44.172	17.492	1.00	18.07
15673	CB	BASN	D	207	-38.221	-44.873	18.770	0.35	18.05
15674	CB	AASN	D	207	-38.252	-44.837	18.793	0.65	18.37
15679	CG	BASN	D	207	-38.785	-46.282	18.925	0.35	18.69
15680	CG	AASN	D	207	-36.860	-45.412	18.699	0.65	19.79
15681	OD1	BASN	D	207	-39.097	-46.954	17.942	0.35	20.02
15682	OD1	AASN	D	207	-36.567	-46.204	17.808	0.65	22.75
15683	ND2	BASN	D	207	-38.905	-46.738	20.167	0.35	18.75
15684	ND2	AASN	D	207	-35.994	-45.029	19.636	0.65	22.52
15689	C	ASN	D	207	-40.145	-43.664	17.648	1.00	17.20
15690	O	ASN	D	207	-40.779	-43.874	18.677	1.00	17.66
15691	N	VAL	D	208	-40.642	-42.989	16.614	1.00	16.47
15693	CA	VAL	D	208	-42.025	-42.526	16.561	1.00	15.54
15695	CB	VAL	D	208	-42.106	-40.986	16.415	1.00	15.82
15697	CG1	VAL	D	208	-43.551	-40.522	16.238	1.00	14.94
15701	CG2	VAL	D	208	-41.478	-40.294	17.629	1.00	16.11
15705	C	VAL	D	208	-42.683	-43.202	15.362	1.00	15.04
15706	O	VAL	D	208	-42.204	-43.075	14.233	1.00	15.24
15707	N	SER	D	209	-43.763	-43.928	15.601	1.00	14.11
15709	CA	SER	D	209	-44.434	-44.658	14.530	1.00	14.39
15711	CB	SER	D	209	-45.128	-45.914	15.057	1.00	14.21
15714	OG	SER	D	209	-46.143	-45.605	15.990	1.00	14.94
15716	C	SER	D	209	-45.431	-43.758	13.818	1.00	14.20
15717	O	SER	D	209	-45.947	-42.809	14.399	1.00	14.77
15718	N	ILE	D	210	-45.666	-44.060	12.542	1.00	14.11
15720	CA	ILE	D	210	-46.611	-43.341	11.697	1.00	14.23
15722	CB	ILE	D	210	-45.873	-42.521	10.613	1.00	14.43
15724	CG1	ILE	D	210	-45.091	-41.396	11.282	1.00	14.25
15727	CD1	ILE	D	210	-44.229	-40.633	10.357	1.00	15.80
15731	CG2	ILE	D	210	-46.850	-41.953	9.572	1.00	14.89
15735	C	ILE	D	210	-47.519	-44.375	11.048	1.00	13.99

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
15736	O	ILE	D	210	-47.054	-45.263	10.318	1.00	13.56
15737	N	THR	D	211	-48.812	-44.245	11.309	1.00	13.21
15739	CA	THR	D	211	-49.834	-45.125	10.773	1.00	13.49
15741	CB	THR	D	211	-50.634	-45.743	11.935	1.00	13.70
15743	OG1	THR	D	211	-49.760	-46.525	12.760	1.00	13.38
15745	CG2	THR	D	211	-51.696	-46.716	11.433	1.00	14.76
15749	C	THR	D	211	-50.772	-44.318	9.882	1.00	13.64
15750	O	THR	D	211	-51.378	-43.361	10.339	1.00	13.82
15751	N	LEU	D	212	-50.907	-44.718	8.623	1.00	13.10
15753	CA	LEU	D	212	-51.856	-44.112	7.696	1.00	13.33
15755	CB	LEU	D	212	-51.186	-43.892	6.347	1.00	13.13
15758	CG	LEU	D	212	-51.994	-43.193	5.250	1.00	14.37
15760	CD1	LEU	D	212	-51.284	-43.309	3.901	1.00	15.55
15764	CD2	LEU	D	212	-52.202	-41.749	5.615	1.00	14.66
15768	C	LEU	D	212	-53.059	-45.029	7.533	1.00	13.73
15769	O	LEU	D	212	-52.911	-46.205	7.187	1.00	14.60
15770	N	CYS	D	213	-54.249	-44.491	7.767	1.00	14.08
15772	CA	CYS	D	213	-55.476	-45.285	7.727	1.00	14.92
15774	CB	CYS	D	213	-56.360	-44.952	8.924	1.00	15.42
15777	SG	CYS	D	213	-55.502	-45.181	10.483	1.00	19.33
15778	C	CYS	D	213	-56.217	-44.987	6.436	1.00	14.38
15779	O	CYS	D	213	-56.367	-43.832	6.065	1.00	15.63
15780	N	VAL	D	214	-56.670	-46.026	5.745	1.00	12.86
15782	CA	VAL	D	214	-57.339	-45.870	4.468	1.00	12.62
15784	CB	VAL	D	214	-56.549	-46.596	3.355	1.00	12.18
15786	CG1	VAL	D	214	-57.284	-46.540	2.019	1.00	12.93
15790	CG2	VAL	D	214	-55.127	-45.994	3.229	1.00	12.88
15794	C	VAL	D	214	-58.746	-46.431	4.622	1.00	12.42
15795	O	VAL	D	214	-58.937	-47.645	4.756	1.00	12.47
15796	N	LEU	D	215	-59.730	-45.531	4.603	1.00	12.02
15798	CA	LEU	D	215	-61.112	-45.871	4.929	1.00	12.50
15800	CB	LEU	D	215	-61.646	-44.900	5.984	1.00	12.51
15803	CG	LEU	D	215	-60.810	-44.662	7.233	1.00	13.93
15805	CD1	LEU	D	215	-61.567	-43.724	8.150	1.00	14.49
15809	CD2	LEU	D	215	-60.428	-45.943	7.935	1.00	14.92
15813	C	LEU	D	215	-62.044	-45.838	3.734	1.00	12.15
15814	O	LEU	D	215	-62.002	-44.910	2.911	1.00	11.97
15815	N	GLY	D	216	-62.897	-46.854	3.652	1.00	12.21
15817	CA	GLY	D	216	-64.020	-46.871	2.732	1.00	12.53
15820	C	GLY	D	216	-65.200	-46.140	3.329	1.00	12.77
15821	O	GLY	D	216	-65.027	-45.317	4.214	1.00	12.73
15822	N	LEU	D	217	-66.400	-46.459	2.857	1.00	12.66
15824	CA	LEU	D	217	-67.601	-45.761	3.312	1.00	13.14
15826	CB	LEU	D	217	-68.787	-46.087	2.407	1.00	13.31
15829	CG	LEU	D	217	-70.150	-45.504	2.796	1.00	13.13
15831	CD1	LEU	D	217	-70.066	-43.993	2.873	1.00	14.01
15835	CD2	LEU	D	217	-71.192	-45.934	1.797	1.00	13.73
15839	C	LEU	D	217	-67.902	-46.169	4.756	1.00	13.52
15840	O	LEU	D	217	-68.069	-47.358	5.057	1.00	13.32

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
15841	N	ILE	D	218	-67.944	-45.178	5.638	1.00	13.96
15843	CA	ILE	D	218	-68.237	-45.348	7.062	1.00	13.92
15845	CB	ILE	D	218	-67.084	-44.799	7.931	1.00	14.20
15847	CG1	ILE	D	218	-65.703	-45.210	7.397	1.00	14.34
15850	CD1	ILE	D	218	-65.460	-46.699	7.257	1.00	14.91
15854	CG2	ILE	D	218	-67.255	-45.226	9.384	1.00	13.90
15858	C	ILE	D	218	-69.511	-44.573	7.394	1.00	14.22
15859	O	ILE	D	218	-69.699	-43.460	6.920	1.00	14.46
15860	N	ASP	D	219	-70.363	-45.142	8.240	1.00	14.52
15862	CA	ASP	D	219	-71.723	-44.613	8.417	1.00	15.08
15864	CB	ASP	D	219	-72.644	-45.738	8.894	1.00	15.09
15867	CG	ASP	D	219	-72.327	-46.213	10.302	1.00	17.19
15868	OD1	ASP	D	219	-73.049	-47.116	10.792	1.00	19.09
15869	OD2	ASP	D	219	-71.402	-45.747	11.000	1.00	18.74
15870	C	ASP	D	219	-71.850	-43.378	9.325	1.00	15.07
15871	O	ASP	D	219	-72.815	-43.257	10.100	1.00	15.22
15872	N	THR	D	220	-70.904	-42.450	9.236	1.00	14.64
15874	CA	THR	D	220	-71.039	-41.178	9.928	1.00	14.25
15876	CB	THR	D	220	-69.729	-40.352	9.895	1.00	14.12
15878	OG1	THR	D	220	-69.416	-39.986	8.541	1.00	13.68
15880	CG2	THR	D	220	-68.550	-41.173	10.373	1.00	14.11
15884	C	THR	D	220	-72.164	-40.368	9.301	1.00	14.78
15885	O	THR	D	220	-72.489	-40.532	8.126	1.00	14.49
15886	N	GLU	D	221	-72.761	-39.482	10.086	1.00	15.44
15888	CA	GLU	D	221	-73.832	-38.644	9.563	1.00	16.66
15890	CB	GLU	D	221	-74.313	-37.659	10.618	1.00	17.41
15893	CG	GLU	D	221	-75.689	-37.090	10.317	1.00	22.02
15896	CD	GLU	D	221	-76.816	-37.980	10.823	1.00	27.19
15897	OE1	GLU	D	221	-77.208	-38.926	10.098	1.00	31.07
15898	OE2	GLU	D	221	-77.311	-37.736	11.952	1.00	32.07
15899	C	GLU	D	221	-73.397	-37.879	8.322	1.00	16.07
15900	O	GLU	D	221	-74.151	-37.758	7.364	1.00	16.20
15901	N	THR	D	222	-72.183	-37.346	8.361	1.00	15.83
15903	CA	THR	D	222	-71.620	-36.625	7.224	1.00	15.25
15905	CB	THR	D	222	-70.178	-36.193	7.569	1.00	15.21
15907	OG1	THR	D	222	-70.208	-35.109	8.511	1.00	15.44
15909	CG2	THR	D	222	-69.467	-35.640	6.358	1.00	15.60
15913	C	THR	D	222	-71.627	-37.474	5.950	1.00	15.08
15914	O	THR	D	222	-72.069	-37.027	4.896	1.00	14.97
15915	N	ALA	D	223	-71.121	-38.694	6.052	1.00	14.99
15917	CA	ALA	D	223	-71.031	-39.582	4.900	1.00	15.06
15919	CB	ALA	D	223	-70.229	-40.819	5.255	1.00	15.15
15923	C	ALA	D	223	-72.401	-39.981	4.385	1.00	15.73
15924	O	ALA	D	223	-72.640	-39.983	3.181	1.00	14.76
15925	N	MET	D	224	-73.307	-40.302	5.300	1.00	16.17
15927	CA	MET	D	224	-74.626	-40.784	4.900	1.00	17.25
15929	CB	MET	D	224	-75.391	-41.333	6.102	1.00	17.89
15932	CG	MET	D	224	-74.723	-42.553	6.741	1.00	19.97
15935	SD	MET	D	224	-74.384	-43.936	5.612	1.00	25.84

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
15936	CE	MET	D	224	-72.839	-43.553	4.977	1.00	27.00
15940	C	MET	D	224	-75.413	-39.691	4.181	1.00	17.30
15941	O	MET	D	224	-76.148	-39.972	3.239	1.00	17.46
15942	N	LYS	D	225	-75.226	-38.444	4.597	1.00	17.77
15944	CA	LYS	D	225	-75.851	-37.316	3.911	1.00	18.38
15946	CB	LYS	D	225	-75.774	-36.058	4.768	1.00	18.96
15949	CG	LYS	D	225	-76.777	-36.054	5.920	1.00	21.88
15952	CD	LYS	D	225	-76.804	-34.699	6.601	1.00	25.58
15955	CE	LYS	D	225	-77.456	-34.743	7.979	1.00	27.29
15958	NZ	LYS	D	225	-76.676	-33.933	8.960	1.00	29.17
15962	C	LYS	D	225	-75.203	-37.080	2.548	1.00	18.03
15963	O	LYS	D	225	-75.888	-36.790	1.572	1.00	17.74
15964	N	ALA	D	226	-73.885	-37.252	2.472	1.00	17.80
15966	CA	ALA	D	226	-73.154	-36.949	1.250	1.00	17.82
15968	CB	ALA	D	226	-71.658	-36.911	1.535	1.00	17.65
15972	C	ALA	D	226	-73.461	-37.947	0.136	1.00	17.96
15973	O	ALA	D	226	-73.466	-37.577	-1.040	1.00	18.22
15974	N	VAL	D	227	-73.722	-39.202	0.501	1.00	18.27
15976	CA	VAL	D	227	-73.970	-40.263	-0.483	1.00	19.00
15978	CB	VAL	D	227	-73.167	-41.554	-0.150	1.00	18.90
15980	CG1	VAL	D	227	-71.706	-41.222	0.084	1.00	19.57
15984	CG2	VAL	D	227	-73.747	-42.284	1.063	1.00	18.40
15988	C	VAL	D	227	-75.452	-40.622	-0.633	1.00	20.12
15989	O	VAL	D	227	-75.793	-41.626	-1.262	1.00	20.83
15990	N	SER	D	228	-76.338	-39.811	-0.063	1.00	20.75
15992	CA	SER	D	228	-77.759	-40.155	-0.055	1.00	21.65
15994	CB	SER	D	228	-78.553	-39.178	0.823	1.00	21.79
15997	OG	SER	D	228	-78.616	-37.897	0.231	1.00	23.95
15999	C	SER	D	228	-78.343	-40.218	-1.465	1.00	22.24
16000	O	SER	D	228	-79.305	-40.965	-1.695	1.00	23.25
16001	N	MET	D	233	-74.403	-48.276	-1.613	1.00	32.20
16003	CA	MET	D	233	-73.673	-49.450	-1.147	1.00	32.18
16005	CB	MET	D	233	-72.276	-49.484	-1.765	1.00	32.75
16008	CG	MET	D	233	-71.391	-48.313	-1.374	1.00	34.20
16011	SD	MET	D	233	-69.887	-48.247	-2.359	1.00	37.48
16012	CE	MET	D	233	-70.391	-47.128	-3.666	1.00	37.54
16016	C	MET	D	233	-73.585	-49.489	0.382	1.00	31.31
16017	O	MET	D	233	-73.984	-48.539	1.066	1.00	31.55
16018	N	GLN	D	234	-73.066	-50.595	0.908	1.00	30.00
16020	CA	GLN	D	234	-73.044	-50.832	2.349	1.00	29.13
16022	CB	GLN	D	234	-72.773	-52.315	2.659	1.00	29.61
16025	CG	GLN	D	234	-74.046	-53.190	2.690	1.00	31.73
16028	CD	GLN	D	234	-74.000	-54.386	1.750	1.00	33.97
16029	OE1	GLN	D	234	-73.053	-54.546	0.978	1.00	36.91
16030	NE2	GLN	D	234	-75.030	-55.229	1.813	1.00	35.97
16033	C	GLN	D	234	-72.016	-49.948	3.056	1.00	27.21
16034	O	GLN	D	234	-70.882	-49.793	2.590	1.00	27.17
16035	N	ALA	D	235	-72.436	-49.358	4.173	1.00	24.83
16037	CA	ALA	D	235	-71.572	-48.496	4.974	1.00	23.17

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
16039	CB	ALA	D	235	-72.295	-47.213	5.346	1.00	22.94
16043	C	ALA	D	235	-71.139	-49.245	6.224	1.00	21.92
16044	O	ALA	D	235	-71.961	-49.854	6.912	1.00	21.77
16045	N	ALA	D	236	-69.849	-49.190	6.518	1.00	20.27
16047	CA	ALA	D	236	-69.296	-49.850	7.692	1.00	19.25
16049	CB	ALA	D	236	-67.811	-50.012	7.535	1.00	19.24
16053	C	ALA	D	236	-69.601	-49.048	8.949	1.00	18.49
16054	O	ALA	D	236	-69.701	-47.829	8.891	1.00	17.77
16055	N	PRO	D	237	-69.734	-49.727	10.087	1.00	17.54
16056	CA	PRO	D	237	-70.028	-49.049	11.348	1.00	17.44
16058	CB	PRO	D	237	-70.346	-50.204	12.312	1.00	17.50
16061	CG	PRO	D	237	-69.702	-51.393	11.736	1.00	17.90
16064	CD	PRO	D	237	-69.604	-51.185	10.256	1.00	17.72
16067	C	PRO	D	237	-68.859	-48.213	11.870	1.00	17.09
16068	O	PRO	D	237	-67.731	-48.703	11.972	1.00	16.60
16069	N	LYS	D	238	-69.157	-46.968	12.224	1.00	16.87
16071	CA	LYS	D	238	-68.155	-46.019	12.699	1.00	16.99
16073	CB	LYS	D	238	-68.766	-44.610	12.819	1.00	16.81
16076	CG	LYS	D	238	-69.951	-44.499	13.790	1.00	17.32
16079	CD	LYS	D	238	-70.707	-43.192	13.617	1.00	17.30
16082	CE	LYS	D	238	-71.748	-43.001	14.717	1.00	19.10
16085	NZ	LYS	D	238	-72.539	-41.754	14.522	1.00	20.29
16089	C	LYS	D	238	-67.494	-46.440	14.010	1.00	16.95
16090	O	LYS	D	238	-66.341	-46.114	14.243	1.00	16.41
16091	N	GLU	D	239	-68.213	-47.161	14.873	1.00	17.55
16093	CA	GLU	D	239	-67.628	-47.645	16.124	1.00	18.48
16095	CB	GLU	D	239	-68.686	-48.311	17.016	1.00	19.09
16098	CG	GLU	D	239	-68.208	-48.592	18.431	1.00	22.45
16101	CD	GLU	D	239	-69.274	-49.242	19.303	1.00	26.03
16102	OE1	GLU	D	239	-68.997	-50.319	19.871	1.00	29.18
16103	OE2	GLU	D	239	-70.389	-48.677	19.431	1.00	30.49
16104	C	GLU	D	239	-66.502	-48.634	15.873	1.00	18.14
16105	O	GLU	D	239	-65.435	-48.533	16.476	1.00	18.30
16106	N	GLU	D	240	-66.748	-49.594	14.986	1.00	18.25
16108	CA	GLU	D	240	-65.738	-50.584	14.615	1.00	18.29
16110	CB	GLU	D	240	-66.365	-51.674	13.749	1.00	18.87
16113	CG	GLU	D	240	-65.419	-52.805	13.384	1.00	21.26
16116	CD	GLU	D	240	-66.119	-53.952	12.676	1.00	25.00
16117	OE1	GLU	D	240	-66.033	-54.036	11.428	1.00	26.25
16118	OE2	GLU	D	240	-66.753	-54.781	13.369	1.00	29.27
16119	C	GLU	D	240	-64.561	-49.946	13.868	1.00	17.26
16120	O	GLU	D	240	-63.404	-50.297	14.103	1.00	16.68
16121	N	CYS	D	241	-64.866	-49.020	12.966	1.00	16.24
16123	CA	CYS	D	241	-63.839	-48.280	12.226	1.00	15.92
16125	CB	CYS	D	241	-64.501	-47.211	11.349	1.00	16.00
16128	SG	CYS	D	241	-63.317	-46.255	10.384	1.00	16.10
16129	C	CYS	D	241	-62.873	-47.601	13.187	1.00	15.63
16130	O	CYS	D	241	-61.659	-47.713	13.070	1.00	14.64
16131	N	ALA	D	242	-63.435	-46.876	14.142	1.00	15.18

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
16133	CA	ALA	D	242	-62.659	-46.170	15.147	1.00	15.69
16135	CB	ALA	D	242	-63.600	-45.457	16.120	1.00	15.70
16139	C	ALA	D	242	-61.729	-47.110	15.897	1.00	15.82
16140	O	ALA	D	242	-60.574	-46.782	16.144	1.00	15.16
16141	N	LEU	D	243	-62.243	-48.276	16.280	1.00	16.06
16143	CA	LEU	D	243	-61.449	-49.227	17.042	1.00	16.56
16145	CB	LEU	D	243	-62.301	-50.396	17.534	1.00	17.39
16148	CG	LEU	D	243	-61.546	-51.427	18.371	1.00	18.77
16150	CD1	LEU	D	243	-60.916	-50.797	19.597	1.00	19.77
16154	CD2	LEU	D	243	-62.482	-52.558	18.773	1.00	20.04
16158	C	LEU	D	243	-60.284	-49.748	16.222	1.00	16.27
16159	O	LEU	D	243	-59.200	-49.861	16.741	1.00	15.92
16160	N	GLU	D	244	-60.516	-50.060	14.947	1.00	16.39
16162	CA	GLU	D	244	-59.455	-50.565	14.076	1.00	16.54
16164	CB	GLU	D	244	-60.026	-51.060	12.751	1.00	17.05
16167	CG	GLU	D	244	-60.889	-52.303	12.881	1.00	18.54
16170	CD	GLU	D	244	-60.158	-53.478	13.510	1.00	22.44
16171	OE1	GLU	D	244	-60.701	-54.060	14.467	1.00	26.15
16172	OE2	GLU	D	244	-59.042	-53.817	13.056	1.00	24.68
16173	C	GLU	D	244	-58.362	-49.541	13.832	1.00	15.87
16174	O	GLU	D	244	-57.201	-49.905	13.689	1.00	16.04
16175	N	ILE	D	245	-58.721	-48.263	13.826	1.00	15.56
16177	CA	ILE	D	245	-57.730	-47.190	13.706	1.00	15.17
16179	CB	ILE	D	245	-58.418	-45.823	13.501	1.00	14.93
16181	CG1	ILE	D	245	-59.069	-45.774	12.114	1.00	15.36
16184	CD1	ILE	D	245	-59.999	-44.603	11.897	1.00	15.56
16188	CG2	ILE	D	245	-57.416	-44.666	13.682	1.00	14.25
16192	C	ILE	D	245	-56.817	-47.182	14.937	1.00	15.76
16193	O	ILE	D	245	-55.588	-47.157	14.814	1.00	15.56
16194	N	ILE	D	246	-57.422	-47.250	16.117	1.00	15.62
16196	CA	ILE	D	246	-56.680	-47.258	17.380	1.00	16.09
16198	CB	ILE	D	246	-57.649	-47.182	18.575	1.00	16.40
16200	CG1	ILE	D	246	-58.318	-45.804	18.643	1.00	16.72
16203	CD1	ILE	D	246	-59.616	-45.782	19.452	1.00	18.04
16207	CG2	ILE	D	246	-56.935	-47.458	19.906	1.00	16.63
16211	C	ILE	D	246	-55.791	-48.490	17.486	1.00	15.95
16212	O	ILE	D	246	-54.645	-48.384	17.906	1.00	16.39
16213	N	LYS	D	247	-56.314	-49.645	17.094	1.00	16.30
16215	CA	LYS	D	247	-55.540	-50.887	17.121	1.00	17.05
16217	CB	LYS	D	247	-56.383	-52.073	16.649	1.00	17.48
16220	CG	LYS	D	247	-57.436	-52.541	17.630	1.00	19.90
16223	CD	LYS	D	247	-57.925	-53.931	17.255	1.00	23.08
16226	CE	LYS	D	247	-59.383	-54.139	17.593	1.00	25.04
16229	NZ	LYS	D	247	-59.795	-55.553	17.367	1.00	26.27
16233	C	LYS	D	247	-54.289	-50.779	16.247	1.00	16.81
16234	O	LYS	D	247	-53.200	-51.153	16.661	1.00	16.63
16235	N	GLY	D	248	-54.454	-50.257	15.039	1.00	16.92
16237	CA	GLY	D	248	-53.341	-50.092	14.125	1.00	17.02
16240	C	GLY	D	248	-52.269	-49.169	14.654	1.00	16.90

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
16241	O	GLY	D	248	-51.081	-49.474	14.546	1.00	17.20
16242	N	GLY	D	249	-52.680	-48.036	15.223	1.00	16.41
16244	CA	GLY	D	249	-51.747	-47.100	15.813	1.00	16.06
16247	C	GLY	D	249	-51.014	-47.717	16.989	1.00	15.69
16248	O	GLY	D	249	-49.796	-47.596	17.101	1.00	16.01
16249	N	ALA	D	250	-51.759	-48.394	17.858	1.00	15.79
16251	CA	ALA	D	250	-51.186	-49.016	19.051	1.00	16.02
16253	CB	ALA	D	250	-52.279	-49.611	19.914	1.00	16.19
16257	C	ALA	D	250	-50.167	-50.089	18.679	1.00	16.03
16258	O	ALA	D	250	-49.136	-50.225	19.342	1.00	16.78
16259	N	LEU	D	251	-50.454	-50.831	17.612	1.00	15.83
16261	CA	LEU	D	251	-49.559	-51.876	17.111	1.00	15.55
16263	CB	LEU	D	251	-50.360	-52.988	16.418	1.00	15.72
16266	CG	LEU	D	251	-51.306	-53.772	17.334	1.00	16.71
16268	CD1	LEU	D	251	-52.111	-54.757	16.508	1.00	18.19
16272	CD2	LEU	D	251	-50.536	-54.485	18.440	1.00	17.97
16276	C	LEU	D	251	-48.481	-51.348	16.158	1.00	15.20
16277	O	LEU	D	251	-47.680	-52.120	15.641	1.00	15.15
16278	N	ARG	D	252	-48.460	-50.039	15.941	1.00	14.81
16280	CA	ARG	D	252	-47.419	-49.370	15.150	1.00	15.10
16282	CB	ARG	D	252	-46.051	-49.450	15.854	1.00	15.46
16285	CG	ARG	D	252	-46.094	-49.004	17.304	1.00	15.63
16288	CD	ARG	D	252	-44.805	-49.174	18.045	1.00	15.97
16291	NE	ARG	D	252	-43.856	-48.087	17.821	1.00	15.98
16293	CZ	ARG	D	252	-43.881	-46.909	18.448	1.00	16.54
16294	NH1	ARG	D	252	-44.829	-46.617	19.341	1.00	16.68
16297	NH2	ARG	D	252	-42.943	-46.012	18.182	1.00	16.88
16300	C	ARG	D	252	-47.336	-49.887	13.712	1.00	15.16
16301	O	ARG	D	252	-46.261	-49.938	13.126	1.00	14.65
16302	N	GLN	D	253	-48.485	-50.269	13.159	1.00	15.44
16304	CA	GLN	D	253	-48.597	-50.675	11.766	1.00	15.82
16306	CB	GLN	D	253	-49.981	-51.279	11.501	1.00	16.25
16309	CG	GLN	D	253	-50.278	-52.555	12.264	1.00	18.91
16312	CD	GLN	D	253	-51.706	-53.028	12.057	1.00	20.15
16313	OE1	GLN	D	253	-52.383	-52.604	11.116	1.00	25.34
16314	NE2	GLN	D	253	-52.167	-53.904	12.929	1.00	24.87
16317	C	GLN	D	253	-48.397	-49.472	10.838	1.00	15.51
16318	O	GLN	D	253	-48.758	-48.351	11.191	1.00	15.60
16319	N	GLU	D	254	-47.839	-49.690	9.656	1.00	15.34
16321	CA	GLU	D	254	-47.654	-48.587	8.707	1.00	15.93
16323	CB	GLU	D	254	-46.739	-48.969	7.544	1.00	16.58
16326	CG	GLU	D	254	-45.283	-49.106	7.938	1.00	19.44
16329	CD	GLU	D	254	-44.310	-49.084	6.767	1.00	22.84
16330	OE1	GLU	D	254	-43.100	-49.214	7.021	1.00	27.77
16331	OE2	GLU	D	254	-44.732	-48.946	5.606	1.00	29.24
16332	C	GLU	D	254	-48.998	-48.120	8.172	1.00	15.32
16333	O	GLU	D	254	-49.231	-46.920	8.040	1.00	14.61
16334	N	GLU	D	255	-49.876	-49.070	7.854	1.00	15.71
16336	CA	GLU	D	255	-51.158	-48.743	7.237	1.00	16.36

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
16338	CB	GLU	D	255	-51.082	-48.830	5.695	1.00	16.58
16341	CG	GLU	D	255	-50.077	-47.843	5.087	1.00	18.91
16344	CD	GLU	D	255	-50.150	-47.698	3.568	1.00	22.25
16345	OE1	GLU	D	255	-49.788	-46.608	3.052	1.00	23.78
16346	OE2	GLU	D	255	-50.527	-48.668	2.880	1.00	25.14
16347	C	GLU	D	255	-52.275	-49.628	7.789	1.00	16.75
16348	O	GLU	D	255	-52.050	-50.805	8.106	1.00	17.67
16349	N	VAL	D	256	-53.452	-49.030	7.938	1.00	16.18
16351	CA	VAL	D	256	-54.688	-49.712	8.294	1.00	16.75
16353	CB	VAL	D	256	-55.330	-49.087	9.546	1.00	17.02
16355	CG1	VAL	D	256	-56.705	-49.697	9.829	1.00	17.92
16359	CG2	VAL	D	256	-54.409	-49.239	10.737	1.00	18.68
16363	C	VAL	D	256	-55.644	-49.539	7.126	1.00	16.45
16364	O	VAL	D	256	-55.812	-48.434	6.631	1.00	17.24
16365	N	TYR	D	257	-56.268	-50.623	6.687	1.00	15.73
16367	CA	TYR	D	257	-57.284	-50.575	5.648	1.00	15.63
16369	CB	TYR	D	257	-56.874	-51.461	4.473	1.00	16.29
16372	CG	TYR	D	257	-55.704	-50.880	3.714	1.00	17.03
16373	CD1	TYR	D	257	-54.398	-51.197	4.052	1.00	20.46
16375	CE1	TYR	D	257	-53.319	-50.634	3.347	1.00	19.65
16377	CZ	TYR	D	257	-53.559	-49.755	2.315	1.00	19.78
16378	OH	TYR	D	257	-52.506	-49.191	1.606	1.00	21.01
16380	CE2	TYR	D	257	-54.845	-49.432	1.968	1.00	18.55
16382	CD2	TYR	D	257	-55.910	-49.987	2.672	1.00	19.21
16384	C	TYR	D	257	-58.596	-51.057	6.247	1.00	15.08
16385	O	TYR	D	257	-58.644	-52.139	6.828	1.00	15.18
16386	N	TYR	D	258	-59.657	-50.265	6.116	1.00	14.26
16388	CA	TYR	D	258	-60.935	-50.604	6.733	1.00	14.38
16390	CB	TYR	D	258	-61.120	-49.887	8.088	1.00	14.66
16393	CG	TYR	D	258	-62.410	-50.303	8.741	1.00	15.21
16394	CD1	TYR	D	258	-63.555	-49.549	8.566	1.00	16.15
16396	CE1	TYR	D	258	-64.746	-49.929	9.119	1.00	18.18
16398	CZ	TYR	D	258	-64.825	-51.091	9.851	1.00	18.07
16399	OH	TYR	D	258	-66.043	-51.452	10.391	1.00	20.65
16401	CE2	TYR	D	258	-63.704	-51.875	10.035	1.00	16.97
16403	CD2	TYR	D	258	-62.503	-51.481	9.472	1.00	16.41
16405	C	TYR	D	258	-62.100	-50.292	5.794	1.00	14.27
16406	O	TYR	D	258	-62.230	-49.178	5.286	1.00	14.30
16407	N	ASP	D	259	-62.953	-51.287	5.592	1.00	14.28
16409	CA	ASP	D	259	-64.089	-51.201	4.685	1.00	14.94
16411	CB	ASP	D	259	-63.626	-51.381	3.235	1.00	15.16
16414	CG	ASP	D	259	-64.712	-51.055	2.212	1.00	16.58
16415	OD1	ASP	D	259	-65.311	-51.988	1.605	1.00	17.34
16416	OD2	ASP	D	259	-65.018	-49.889	1.932	1.00	18.72
16417	C	ASP	D	259	-65.052	-52.329	5.019	1.00	15.18
16418	O	ASP	D	259	-64.672	-53.313	5.648	1.00	15.59
16419	N	SER	D	260	-66.285	-52.200	4.559	1.00	15.42
16421	CA	SER	D	260	-67.278	-53.260	4.724	1.00	16.09
16423	CB	BSER	D	260	-68.629	-52.816	4.156	0.35	16.09



## FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
16424	CB	ASER	D	260	-68.642	-52.796	4.199	0.65	16.44
16429	OG	BSER	D	260	-69.192	-51.779	4.933	0.35	15.90
16430	OG	ASER	D	260	-68.618	-52.596	2.800	0.65	18.35
16433	C	SER	D	260	-66.855	-54.567	4.046	1.00	16.08
16434	O	SER	D	260	-67.272	-55.643	4.478	1.00	16.88
16435	N	SER	D	261	-66.038	-54.478	2.997	1.00	16.11
16437	CA	SER	D	261	-65.723	-55.646	2.180	1.00	16.14
16439	CB	SER	D	261	-66.192	-55.417	0.751	1.00	16.57
16442	OG	SER	D	261	-65.776	-56.501	-0.070	1.00	17.84
16444	C	SER	D	261	-64.235	-55.962	2.159	1.00	15.61
16445	O	SER	D	261	-63.413	-55.077	1.998	1.00	14.84
16446	N	LEU	D	262	-63.912	-57.241	2.296	1.00	15.67
16448	CA	LEU	D	262	-62.542	-57.716	2.134	1.00	15.58
16450	CB	LEU	D	262	-62.425	-59.186	2.560	1.00	16.01
16453	CG	LEU	D	262	-62.414	-59.390	4.077	1.00	17.84
16455	CD1	LEU	D	262	-62.557	-60.855	4.432	1.00	19.74
16459	CD2	LEU	D	262	-61.144	-58.789	4.696	1.00	20.46
16463	C	LEU	D	262	-62.034	-57.547	0.706	1.00	15.03
16464	O	LEU	D	262	-60.825	-57.499	0.489	1.00	14.66
16465	N	TRP	D	263	-62.933	-57.493	-0.275	1.00	14.43
16467	CA	TRP	D	263	-62.519	-57.213	-1.647	1.00	14.54
16469	CB	TRP	D	263	-63.708	-57.244	-2.609	1.00	14.72
16472	CG	TRP	D	263	-64.184	-58.633	-2.909	1.00	13.81
16473	CD1	TRP	D	263	-64.952	-59.420	-2.115	1.00	15.11
16475	NE1	TRP	D	263	-65.173	-60.632	-2.717	1.00	13.92
16477	CE2	TRP	D	263	-64.535	-60.654	-3.928	1.00	13.81
16478	CD2	TRP	D	263	-63.885	-59.411	-4.076	1.00	13.55
16479	CE3	TRP	D	263	-63.162	-59.172	-5.248	1.00	12.56
16481	CZ3	TRP	D	263	-63.081	-60.177	-6.205	1.00	13.80
16483	CH2	TRP	D	263	-63.738	-61.397	-6.027	1.00	13.72
16485	CZ2	TRP	D	263	-64.462	-61.661	-4.895	1.00	13.27
16487	C	TRP	D	263	-61.816	-55.854	-1.692	1.00	14.53
16488	O	TRP	D	263	-60.788	-55.690	-2.338	1.00	15.23
16489	N	THR	D	264	-62.367	-54.888	-0.968	1.00	13.92
16491	CA	THR	D	264	-61.772	-53.561	-0.893	1.00	13.83
16493	CB	THR	D	264	-62.729	-52.580	-0.208	1.00	13.63
16495	OG1	THR	D	264	-63.992	-52.593	-0.878	1.00	15.71
16497	CG2	THR	D	264	-62.213	-51.139	-0.334	1.00	13.64
16501	C	THR	D	264	-60.456	-53.549	-0.145	1.00	14.10
16502	O	THR	D	264	-59.456	-53.082	-0.673	1.00	14.03
16503	N	THR	D	265	-60.450	-54.031	1.096	1.00	14.17
16505	CA	THR	D	265	-59.248	-53.892	1.923	1.00	14.54
16507	CB	THR	D	265	-59.495	-54.251	3.393	1.00	14.50
16509	OG1	THR	D	265	-59.934	-55.603	3.482	1.00	15.19
16511	CG2	THR	D	265	-60.602	-53.385	4.004	1.00	15.04
16515	C	THR	D	265	-58.080	-54.723	1.421	1.00	14.43
16516	O	THR	D	265	-56.938	-54.322	1.601	1.00	15.40
16517	N	LEU	D	266	-58.344	-55.868	0.801	1.00	13.85
16519	CA	LEU	D	266	-57.251	-56.687	0.267	1.00	13.71

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
16521	CB	LEU	D	266	-57.655	-58.166	0.182	1.00	13.50
16524	CG	LEU	D	266	-57.992	-58.840	1.515	1.00	14.59
16526	CD1	LEU	D	266	-58.411	-60.270	1.276	1.00	13.73
16530	CD2	LEU	D	266	-56.823	-58.793	2.502	1.00	16.31
16534	C	LEU	D	266	-56.731	-56.195	-1.084	1.00	13.82
16535	O	LEU	D	266	-55.536	-56.248	-1.317	1.00	14.37
16536	N	LEU	D	267	-57.608	-55.732	-1.970	1.00	13.67
16538	CA	LEU	D	267	-57.182	-55.349	-3.320	1.00	13.99
16540	CB	LEU	D	267	-58.330	-55.507	-4.326	1.00	14.36
16543	CG	LEU	D	267	-58.775	-56.947	-4.600	1.00	14.27
16545	CD1	LEU	D	267	-60.002	-56.962	-5.487	1.00	13.76
16549	CD2	LEU	D	267	-57.645	-57.760	-5.240	1.00	15.52
16553	C	LEU	D	267	-56.583	-53.946	-3.409	1.00	14.41
16554	O	LEU	D	267	-55.782	-53.677	-4.300	1.00	14.45
16555	N	ILE	D	268	-56.960	-53.061	-2.487	1.00	15.23
16557	CA	ILE	D	268	-56.471	-51.678	-2.496	1.00	16.15
16559	CB	ILE	D	268	-57.359	-50.772	-1.602	1.00	16.75
16561	CG1	ILE	D	268	-57.074	-49.293	-1.860	1.00	19.30
16564	CD1	ILE	D	268	-57.467	-48.841	-3.223	1.00	21.79
16568	CG2	ILE	D	268	-57.128	-51.065	-0.134	1.00	18.51
16572	C	ILE	D	268	-55.025	-51.585	-2.039	1.00	16.20
16573	O	ILE	D	268	-54.324	-50.618	-2.361	1.00	15.68
16574	N	ARG	D	269	-54.578	-52.578	-1.284	1.00	17.20
16576	CA	ARG	D	269	-53.202	-52.585	-0.815	1.00	17.96
16578	CB	ARG	D	269	-52.977	-53.664	0.260	1.00	19.69
16581	CG	ARG	D	269	-52.833	-55.080	-0.226	1.00	24.02
16584	CD	ARG	D	269	-53.139	-56.152	0.837	1.00	29.25
16587	NE	ARG	D	269	-52.596	-55.787	2.151	1.00	33.30
16589	CZ	ARG	D	269	-53.308	-55.384	3.210	1.00	35.92
16590	NH1	ARG	D	269	-52.671	-55.078	4.334	1.00	37.17
16593	NH2	ARG	D	269	-54.638	-55.285	3.170	1.00	35.60
16596	C	ARG	D	269	-52.264	-52.735	-2.014	1.00	16.85
16597	O	ARG	D	269	-52.565	-53.441	-2.979	1.00	16.88
16598	N	ASN	D	270	-51.131	-52.045	-1.929	1.00	16.07
16600	CA	ASN	D	270	-50.146	-51.990	-3.002	1.00	15.26
16602	CB	ASN	D	270	-50.113	-50.560	-3.584	1.00	15.13
16605	CG	ASN	D	270	-49.121	-50.383	-4.748	1.00	16.00
16606	OD1	ASN	D	270	-48.871	-49.256	-5.175	1.00	17.02
16607	ND2	ASN	D	270	-48.574	-51.476	-5.262	1.00	14.33
16610	C	ASN	D	270	-48.783	-52.402	-2.449	1.00	15.05
16611	O	ASN	D	270	-47.897	-51.558	-2.243	1.00	14.33
16612	N	PRO	D	271	-48.591	-53.698	-2.196	1.00	14.46
16613	CA	PRO	D	271	-47.327	-54.160	-1.613	1.00	14.37
16615	CB	PRO	D	271	-47.569	-55.662	-1.392	1.00	14.92
16618	CG	PRO	D	271	-48.612	-56.018	-2.341	1.00	14.78
16621	CD	PRO	D	271	-49.524	-54.818	-2.408	1.00	14.82
16624	C	PRO	D	271	-46.129	-53.904	-2.523	1.00	14.44
16625	O	PRO	D	271	-45.024	-53.745	-2.005	1.00	14.26
16626	N	SER	D	272	-46.338	-53.830	-3.838	1.00	14.50

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
16628	CA	SER	D	272	-45.229	-53.577	-4.753	1.00	14.79
16630	CB	SER	D	272	-45.703	-53.643	-6.207	1.00	15.34
16633	OG	SER	D	272	-46.073	-54.968	-6.561	1.00	17.89
16635	C	SER	D	272	-44.578	-52.230	-4.487	1.00	14.61
16636	O	SER	D	272	-43.375	-52.077	-4.649	1.00	13.54
16637	N	ARG	D	273	-45.371	-51.230	-4.113	1.00	15.60
16639	CA	ARG	D	273	-44.797	-49.938	-3.764	1.00	16.01
16641	CB	ARG	D	273	-45.899	-48.921	-3.403	1.00	16.07
16644	CG	ARG	D	273	-45.358	-47.694	-2.710	1.00	15.01
16647	CD	ARG	D	273	-46.370	-46.553	-2.535	1.00	14.64
16650	NE	ARG	D	273	-46.050	-45.782	-1.331	1.00	14.56
16652	CZ	ARG	D	273	-46.860	-44.881	-0.791	1.00	15.26
16653	NH1	ARG	D	273	-48.007	-44.588	-1.362	1.00	14.99
16656	NH2	ARG	D	273	-46.516	-44.270	0.328	1.00	15.71
16659	C	ARG	D	273	-43.794	-50.066	-2.615	1.00	16.24
16660	O	ARG	D	273	-42.690	-49.522	-2.690	1.00	16.48
16661	N	LYS	D	274	-44.178	-50.773	-1.554	1.00	17.53
16663	CA	LYS	D	274	-43.332	-50.918	-0.372	1.00	18.78
16665	CB	LYS	D	274	-44.093	-51.661	0.746	1.00	19.82
16668	CG	LYS	D	274	-45.431	-51.021	1.176	1.00	23.62
16671	CD	LYS	D	274	-46.275	-51.957	2.055	1.00	28.48
16674	CE	LYS	D	274	-45.919	-51.868	3.550	1.00	30.49
16677	NZ	LYS	D	274	-47.100	-51.533	4.423	1.00	31.15
16681	C	LYS	D	274	-42.053	-51.679	-0.732	1.00	18.11
16682	O	LYS	D	274	-40.970	-51.381	-0.227	1.00	17.79
16683	N	ILE	D	275	-42.192	-52.644	-1.629	1.00	18.14
16685	CA	ILE	D	275	-41.054	-53.447	-2.076	1.00	18.22
16687	CB	ILE	D	275	-41.535	-54.657	-2.908	1.00	18.24
16689	CG1	ILE	D	275	-42.146	-55.710	-1.978	1.00	20.23
16692	CD1	ILE	D	275	-43.036	-56.708	-2.670	1.00	22.09
16696	CG2	ILE	D	275	-40.382	-55.260	-3.718	1.00	18.75
16700	C	ILE	D	275	-40.078	-52.589	-2.857	1.00	17.74
16701	O	ILE	D	275	-38.875	-52.624	-2.597	1.00	17.63
16702	N	LEU	D	276	-40.593	-51.801	-3.796	1.00	17.33
16704	CA	LEU	D	276	-39.729	-50.936	-4.600	1.00	17.66
16706	CB	LEU	D	276	-40.500	-50.263	-5.737	1.00	18.11
16709	CG	LEU	D	276	-40.921	-51.167	-6.894	1.00	20.10
16711	CD1	LEU	D	276	-41.724	-50.349	-7.893	1.00	21.41
16715	CD2	LEU	D	276	-39.721	-51.807	-7.576	1.00	20.17
16719	C	LEU	D	276	-39.053	-49.889	-3.728	1.00	17.46
16720	O	LEU	D	276	-37.881	-49.592	-3.916	1.00	17.82
16721	N	GLU	D	277	-39.778	-49.313	-2.767	1.00	17.22
16723	CA	GLU	D	277	-39.150	-48.350	-1.861	1.00	17.40
16725	CB	GLU	D	277	-40.159	-47.815	-0.841	1.00	17.21
16728	CG	GLU	D	277	-41.231	-46.927	-1.464	1.00	17.04
16731	CD	GLU	D	277	-42.411	-46.650	-0.547	1.00	17.50
16732	OE1	GLU	D	277	-43.281	-45.860	-0.960	1.00	15.95
16733	OE2	GLU	D	277	-42.507	-47.206	0.570	1.00	18.68
16734	C	GLU	D	277	-37.959	-48.987	-1.141	1.00	17.92

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
16735	O	GLU	D	277	-36.892	-48.378	-1.018	1.00	18.61
16736	N	PHE	D	278	-38.140	-50.218	-0.687	1.00	19.15
16738	CA	PHE	D	278	-37.058	-50.932	-0.007	1.00	19.63
16740	CB	PHE	D	278	-37.585	-52.224	0.610	1.00	20.25
16743	CG	PHE	D	278	-36.509	-53.121	1.134	1.00	22.47
16744	CD1	PHE	D	278	-35.915	-52.866	2.360	1.00	25.60
16746	CE1	PHE	D	278	-34.911	-53.705	2.847	1.00	27.06
16748	CZ	PHE	D	278	-34.499	-54.795	2.095	1.00	26.78
16750	CE2	PHE	D	278	-35.083	-55.051	0.865	1.00	26.02
16752	CD2	PHE	D	278	-36.083	-54.216	0.391	1.00	24.26
16754	C	PHE	D	278	-35.886	-51.224	-0.954	1.00	20.08
16755	O	PHE	D	278	-34.720	-50.971	-0.614	1.00	20.61
16756	N	LEU	D	279	-36.185	-51.714	-2.154	1.00	20.00
16758	CA	LEU	D	279	-35.139	-52.038	-3.130	1.00	20.48
16760	CB	LEU	D	279	-35.732	-52.754	-4.346	1.00	20.36
16763	CG	LEU	D	279	-36.248	-54.166	-4.042	1.00	19.94
16765	CD1	LEU	D	279	-37.011	-54.761	-5.212	1.00	19.99
16769	CD2	LEU	D	279	-35.107	-55.106	-3.599	1.00	19.70
16773	C	LEU	D	279	-34.343	-50.799	-3.553	1.00	21.44
16774	O	LEU	D	279	-33.124	-50.855	-3.697	1.00	21.55
16775	N	TYR	D	280	-35.030	-49.669	-3.683	1.00	21.51
16777	CA	TYR	D	280	-34.417	-48.408	-4.100	1.00	22.75
16779	CB	TYR	D	280	-35.501	-47.408	-4.505	1.00	22.11
16782	CG	TYR	D	280	-36.240	-47.702	-5.790	1.00	21.31
16783	CD1	TYR	D	280	-37.225	-46.833	-6.240	1.00	20.99
16785	CE1	TYR	D	280	-37.916	-47.071	-7.397	1.00	21.29
16787	CZ	TYR	D	280	-37.658	-48.201	-8.138	1.00	20.57
16788	OH	TYR	D	280	-38.363	-48.442	-9.289	1.00	22.36
16790	CE2	TYR	D	280	-36.682	-49.096	-7.720	1.00	19.70
16792	CD2	TYR	D	280	-35.996	-48.855	-6.543	1.00	20.32
16794	C	TYR	D	280	-33.574	-47.760	-3.011	1.00	24.15
16795	O	TYR	D	280	-32.790	-46.845	-3.306	1.00	26.18
16796	N	SER	D	281	-33.762	-48.178	-1.763	1.00	24.89
16798	CA	SER	D	281	-33.004	-47.617	-0.644	1.00	26.06
16800	CB	SER	D	281	-33.744	-47.839	0.679	1.00	26.00
16803	OG	SER	D	281	-33.716	-49.200	1.078	1.00	27.53
16805	C	SER	D	281	-31.605	-48.224	-0.583	1.00	26.92
16806	O	SER	D	281	-31.401	-49.345	-1.066	1.00	28.17
16807	O2	NAD	E	1	8.751	2.102	17.407	1.00	12.17
16808	C1	NAD	E	1	8.215	1.537	18.361	1.00	12.62
16809	N3	NAD	E	1	8.918	0.857	19.267	1.00	12.48
16812	C4	NAD	E	1	6.722	1.596	18.452	1.00	11.10
16813	C5	NAD	E	1	6.021	2.273	17.473	1.00	12.25
16815	C6	NAD	E	1	4.640	2.351	17.528	1.00	12.56
16817	C7	NAD	E	1	4.000	1.747	18.596	1.00	12.90
16819	C9	NAD	E	1	6.038	0.995	19.498	1.00	12.32
16821	N8	NAD	E	1	4.707	1.091	19.524	1.00	12.37
16822	C10	NAD	E	1	3.967	0.451	20.591	1.00	13.06
16824	C11	NAD	E	1	3.575	-0.985	20.291	1.00	12.60

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
16826	O15	NAD	E	1	2.468	-1.233	19.439	1.00	12.09
16828	C12	NAD	E	1	3.554	-1.648	21.638	1.00	12.74
16830	O16	NAD	E	1	2.181	-1.504	22.014	1.00	11.94
16832	O14	NAD	E	1	4.553	0.491	21.875	1.00	12.96
16833	C13	NAD	E	1	4.302	-0.742	22.582	1.00	12.45
16835	C17	NAD	E	1	5.617	-1.358	23.023	1.00	12.35
16838	O18	NAD	E	1	6.467	-1.539	21.890	1.00	13.48
16839	P19	NAD	E	1	7.989	-2.034	22.131	1.00	12.97
16840	O20	NAD	E	1	8.443	-1.534	23.460	1.00	12.70
16841	O21	NAD	E	1	8.738	-1.691	20.882	1.00	12.69
16842	O22	NAD	E	1	7.766	-3.629	22.169	1.00	13.47
16843	P23	NAD	E	1	8.806	-4.751	22.678	1.00	13.64
16844	O24	NAD	E	1	10.101	-4.134	23.160	1.00	13.15
16845	O25	NAD	E	1	8.871	-5.753	21.582	1.00	14.05
16846	O26	NAD	E	1	8.013	-5.355	23.938	1.00	13.80
16847	C27	NAD	E	1	6.907	-6.234	23.755	1.00	13.48
16850	C28	NAD	E	1	6.493	-6.755	25.124	1.00	11.65
16852	C29	NAD	E	1	7.586	-7.673	25.606	1.00	11.90
16854	O33	NAD	E	1	7.570	-7.539	27.039	1.00	13.89
16856	O32	NAD	E	1	5.292	-7.531	24.977	1.00	13.75
16857	C31	NAD	E	1	5.578	-8.874	25.357	1.00	13.11
16859	C30	NAD	E	1	7.086	-9.059	25.410	1.00	13.17
16861	O34	NAD	E	1	7.656	-10.046	26.257	1.00	14.05
16862	P35	NAD	E	1	7.592	-11.626	25.953	1.00	14.24
16863	O37	NAD	E	1	8.548	-12.192	26.979	1.00	16.17
16864	O36	NAD	E	1	6.170	-12.045	26.181	1.00	14.39
16865	O38	NAD	E	1	8.067	-11.828	24.530	1.00	14.16
16866	N39	NAD	E	1	4.820	-9.904	24.671	1.00	12.28
16867	C40	NAD	E	1	3.782	-10.559	25.156	1.00	12.08
16868	N47	NAD	E	1	3.160	-10.434	26.430	1.00	11.08
16869	C41	NAD	E	1	3.337	-11.502	24.183	1.00	11.01
16870	N42	NAD	E	1	4.137	-11.359	23.121	1.00	12.14
16871	C43	NAD	E	1	5.036	-10.389	23.432	1.00	11.14
16873	C44	NAD	E	1	2.211	-12.337	24.572	1.00	11.86
16874	N48	NAD	E	1	1.745	-13.250	23.693	1.00	12.80
16877	N45	NAD	E	1	1.676	-12.165	25.809	1.00	12.12
16878	C46	NAD	E	1	2.129	-11.258	26.688	1.00	11.72
16880	O2	NAD	E	2	-27.810	2.961	9.373	1.00	13.69
16881	C1	NAD	E	2	-27.399	1.962	8.814	1.00	14.14
16882	N3	NAD	E	2	-28.218	1.072	8.262	1.00	13.27
16885	C4	NAD	E	2	-25.920	1.748	8.754	1.00	13.12
16886	C5	NAD	E	2	-25.089	2.696	9.348	1.00	13.89
16888	C6	NAD	E	2	-23.717	2.526	9.293	1.00	13.22
16890	C7	NAD	E	2	-23.187	1.413	8.671	1.00	12.77
16892	C9	NAD	E	2	-25.355	0.638	8.136	1.00	12.40
16894	N8	NAD	E	2	-24.014	0.504	8.120	1.00	12.22
16895	C10	NAD	E	2	-23.405	-0.657	7.488	1.00	13.86
16897	C11	NAD	E	2	-23.185	-1.831	8.429	1.00	14.57
16899	O15	NAD	E	2	-22.081	-1.793	9.307	1.00	13.40

## FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
16901	C12	NAD	E	2	-23.317	-3.042	7.538	1.00	13.49
16903	O16	NAD	E	2	-21.950	-3.359	7.188	1.00	11.94
16905	O14	NAD	E	2	-24.053	-1.152	6.317	1.00	13.68
16906	C13	NAD	E	2	-23.982	-2.578	6.265	1.00	13.20
16908	C17	NAD	E	2	-25.392	-3.141	6.106	1.00	13.38
16911	O18	NAD	E	2	-26.214	-2.664	7.181	1.00	13.61
16912	P19	NAD	E	2	-27.822	-2.915	7.176	1.00	12.64
16913	O20	NAD	E	2	-28.262	-3.056	5.766	1.00	13.33
16914	O21	NAD	E	2	-28.456	-1.943	8.119	1.00	12.86
16915	O22	NAD	E	2	-27.836	-4.361	7.891	1.00	13.44
16916	P23	NAD	E	2	-29.028	-5.470	7.892	1.00	13.62
16917	O24	NAD	E	2	-30.204	-4.998	7.102	1.00	14.21
16918	O25	NAD	E	2	-29.196	-5.826	9.322	1.00	12.90
16919	O26	NAD	E	2	-28.359	-6.691	7.104	1.00	12.90
16920	C27	NAD	E	2	-27.292	-7.462	7.655	1.00	13.44
16923	C28	NAD	E	2	-27.102	-8.678	6.766	1.00	12.69
16925	C29	NAD	E	2	-28.358	-9.525	6.749	1.00	13.24
16927	O33	NAD	E	2	-28.387	-10.052	5.420	1.00	13.83
16929	O32	NAD	E	2	-26.066	-9.470	7.325	1.00	12.95
16930	C31	NAD	E	2	-26.556	-10.762	7.613	1.00	13.66
16932	C30	NAD	E	2	-28.083	-10.723	7.595	1.00	13.71
16934	O34	NAD	E	2	-28.839	-11.887	7.281	1.00	14.53
16935	P35	NAD	E	2	-29.026	-13.101	8.330	1.00	14.73
16936	O37	NAD	E	2	-30.112	-13.922	7.668	1.00	16.19
16937	O36	NAD	E	2	-27.704	-13.806	8.360	1.00	15.06
16938	O38	NAD	E	2	-29.445	-12.538	9.662	1.00	14.72
16939	N39	NAD	E	2	-25.912	-11.445	8.720	1.00	12.70
16940	C40	NAD	E	2	-25.035	-12.427	8.605	1.00	11.90
16941	N47	NAD	E	2	-24.462	-12.991	7.428	1.00	13.06
16942	C41	NAD	E	2	-24.682	-12.878	9.910	1.00	12.10
16943	N42	NAD	E	2	-25.406	-12.135	10.758	1.00	12.89
16944	C43	NAD	E	2	-26.156	-11.288	10.016	1.00	12.05
16946	C44	NAD	E	2	-23.699	-13.969	9.979	1.00	11.69
16947	N48	NAD	E	2	-23.333	-14.439	11.184	1.00	14.12
16950	N45	NAD	E	2	-23.215	-14.455	8.830	1.00	13.47
16951	C46	NAD	E	2	-23.570	-13.989	7.625	1.00	12.53
16953	O2	NAD	E	3	-34.117	-35.627	-11.946	1.00	13.66
16954	C1	NAD	E	3	-34.853	-34.705	-12.311	1.00	13.42
16955	N3	NAD	E	3	-34.391	-33.677	-13.000	1.00	13.03
16958	C4	NAD	E	3	-36.325	-34.775	-12.001	1.00	11.89
16959	C5	NAD	E	3	-36.792	-35.883	-11.292	1.00	13.56
16961	C6	NAD	E	3	-38.150	-35.997	-11.019	1.00	13.36
16963	C7	NAD	E	3	-39.004	-34.994	-11.439	1.00	13.29
16965	C9	NAD	E	3	-37.223	-33.795	-12.411	1.00	13.42
16967	N8	NAD	E	3	-38.527	-33.950	-12.115	1.00	12.62
16968	C10	NAD	E	3	-39.478	-32.922	-12.488	1.00	13.12
16970	C11	NAD	E	3	-39.697	-31.833	-11.451	1.00	12.65
16972	O15	NAD	E	3	-40.492	-32.108	-10.308	1.00	12.94
16974	C12	NAD	E	3	-40.048	-30.606	-12.267	1.00	11.65

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
16976	O16	NAD	E	3	-41.481	-30.594	-12.282	1.00	12.23
16978	O14	NAD	E	3	-39.247	-32.302	-13.734	1.00	12.68
16979	C13	NAD	E	3	-39.630	-30.914	-13.692	1.00	11.79
16981	C17	NAD	E	3	-38.463	-30.048	-14.145	1.00	13.10
16984	O18	NAD	E	3	-37.335	-30.394	-13.333	1.00	13.65
16985	P19	NAD	E	3	-35.865	-29.854	-13.703	1.00	13.36
16986	O20	NAD	E	3	-35.801	-29.493	-15.150	1.00	13.46
16987	O21	NAD	E	3	-34.884	-30.820	-13.117	1.00	12.89
16988	O22	NAD	E	3	-35.784	-28.527	-12.805	1.00	15.28
16989	P23	NAD	E	3	-34.948	-27.166	-13.045	1.00	15.47
16990	O24	NAD	E	3	-33.908	-27.346	-14.105	1.00	17.48
16991	O25	NAD	E	3	-34.598	-26.666	-11.664	1.00	17.28
16992	O26	NAD	E	3	-36.100	-26.236	-13.662	1.00	14.95
16993	C27	NAD	E	3	-37.149	-25.692	-12.871	1.00	14.37
16996	C28	NAD	E	3	-37.769	-24.568	-13.688	1.00	13.95
16998	C29	NAD	E	3	-36.717	-23.526	-13.973	1.00	13.85
17000	O33	NAD	E	3	-37.009	-23.006	-15.299	1.00	14.30
17002	O32	NAD	E	3	-38.792	-23.952	-12.897	1.00	14.19
17003	C31	NAD	E	3	-38.448	-22.581	-12.675	1.00	13.68
17005	C30	NAD	E	3	-36.997	-22.373	-13.093	1.00	13.48
17007	O34	NAD	E	3	-36.579	-21.148	-13.658	1.00	13.85
17008	P35	NAD	E	3	-36.236	-19.808	-12.833	1.00	14.31
17009	O37	NAD	E	3	-35.744	-18.967	-13.976	1.00	15.22
17010	O36	NAD	E	3	-37.522	-19.353	-12.225	1.00	13.21
17011	O38	NAD	E	3	-35.150	-20.150	-11.825	1.00	15.38
17012	N39	NAD	E	3	-38.813	-22.033	-11.372	1.00	13.30
17013	C40	NAD	E	3	-39.832	-21.216	-11.158	1.00	13.46
17014	N47	NAD	E	3	-40.829	-20.743	-12.058	1.00	12.32
17015	C41	NAD	E	3	-39.851	-20.851	-9.765	1.00	12.36
17016	N42	NAD	E	3	-38.788	-21.452	-9.220	1.00	12.24
17017	C43	NAD	E	3	-38.174	-22.149	-10.198	1.00	12.92
17019	C44	NAD	E	3	-40.943	-19.964	-9.351	1.00	13.46
17020	N48	NAD	E	3	-41.011	-19.582	-8.060	1.00	14.63
17023	N45	NAD	E	3	-41.834	-19.560	-10.272	1.00	13.04
17024	C46	NAD	E	3	-41.770	-19.930	-11.569	1.00	14.15
17026	O2	NAD	E	4	-67.060	-42.510	4.780	1.00	16.74
17027	C1	NAD	E	4	-66.453	-41.855	5.611	1.00	15.31
17028	N3	NAD	E	4	-67.048	-41.410	6.729	1.00	16.22
17031	C4	NAD	E	4	-65.005	-41.585	5.344	1.00	16.29
17032	C5	NAD	E	4	-64.456	-42.091	4.167	1.00	15.48
17034	C6	NAD	E	4	-63.114	-41.870	3.899	1.00	15.41
17036	C7	NAD	E	4	-62.353	-41.156	4.800	1.00	15.97
17038	C9	NAD	E	4	-64.197	-40.879	6.218	1.00	16.21
17040	N8	NAD	E	4	-62.907	-40.676	5.930	1.00	14.62
17041	C10	NAD	E	4	-62.046	-39.930	6.809	1.00	15.56
17043	C11	NAD	E	4	-61.998	-38.436	6.527	1.00	15.57
17045	O15	NAD	E	4	-61.224	-37.948	5.439	1.00	14.99
17047	C12	NAD	E	4	-61.764	-37.799	7.867	1.00	15.11
17049	O16	NAD	E	4	-60.342	-37.609	7.927	1.00	14.75

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
17051	O14	NAD	E	4	-62.284	-40.104	8.215	1.00	15.60
17052	C13	NAD	E	4	-62.093	-38.862	8.912	1.00	15.54
17054	C17	NAD	E	4	-63.364	-38.525	9.697	1.00	16.51
17057	O18	NAD	E	4	-64.479	-38.439	8.821	1.00	16.78
17058	P19	NAD	E	4	-65.984	-38.339	9.412	1.00	17.84
17059	O20	NAD	E	4	-65.939	-38.884	10.808	1.00	17.58
17060	O21	NAD	E	4	-66.912	-38.885	8.382	1.00	17.04
17061	O22	NAD	E	4	-66.124	-36.744	9.475	1.00	18.11
17062	P23	NAD	E	4	-67.212	-35.875	10.324	1.00	19.23
17063	O24	NAD	E	4	-68.227	-36.775	10.969	1.00	21.51
17064	O25	NAD	E	4	-67.695	-34.823	9.372	1.00	19.94
17065	O26	NAD	E	4	-66.270	-35.207	11.407	1.00	17.31
17066	C27	NAD	E	4	-65.320	-34.187	11.061	1.00	18.60
17069	C28	NAD	E	4	-64.731	-33.574	12.309	1.00	18.23
17071	C29	NAD	E	4	-65.859	-32.895	13.051	1.00	18.79
17073	O33	NAD	E	4	-65.545	-33.090	14.431	1.00	19.43
17075	O32	NAD	E	4	-63.792	-32.549	11.971	1.00	18.43
17076	C31	NAD	E	4	-64.237	-31.289	12.470	1.00	18.85
17078	C30	NAD	E	4	-65.680	-31.427	12.899	1.00	19.84
17080	O34	NAD	E	4	-66.101	-30.669	14.011	1.00	21.05
17081	P35	NAD	E	4	-66.765	-29.203	13.874	1.00	22.67
17082	O37	NAD	E	4	-67.399	-29.097	15.242	1.00	26.36
17083	O36	NAD	E	4	-65.539	-28.359	13.794	1.00	23.44
17084	O38	NAD	E	4	-67.672	-29.178	12.675	1.00	23.97
17085	N39	NAD	E	4	-63.932	-30.102	11.665	1.00	17.93
17086	C40	NAD	E	4	-62.995	-29.226	11.950	1.00	16.40
17087	N47	NAD	E	4	-62.062	-29.203	13.038	1.00	17.28
17088	C41	NAD	E	4	-63.017	-28.188	10.952	1.00	16.02
17089	N42	NAD	E	4	-63.996	-28.518	10.110	1.00	16.09
17090	C43	NAD	E	4	-64.553	-29.673	10.551	1.00	16.87
17092	C44	NAD	E	4	-62.015	-27.128	11.155	1.00	17.11
17093	N48	NAD	E	4	-61.957	-26.103	10.276	1.00	18.90
17096	N45	NAD	E	4	-61.176	-27.192	12.206	1.00	17.55
17097	C46	NAD	E	4	-61.203	-28.182	13.123	1.00	16.88
17099	O28	syr	F	1	5.729	7.519	9.589	1.00	16.31
17100	C27	syr	F	1	6.486	7.478	10.557	1.00	16.13
17101	N29	syr	F	1	6.876	8.569	11.198	1.00	15.79
17103	C30	syr	F	1	6.402	9.906	10.874	1.00	18.39
17106	C31	syr	F	1	6.854	10.468	9.532	1.00	20.78
17109	C32	syr	F	1	8.367	10.520	9.432	1.00	23.90
17112	N33	syr	F	1	8.885	11.044	8.149	1.00	25.33
17113	C35	syr	F	1	8.598	10.103	7.047	1.00	25.50
17117	C34	syr	F	1	8.321	12.368	7.806	1.00	25.07
17121	C36	syr	F	1	10.358	11.116	8.245	1.00	30.12
17124	C37	syr	F	1	10.882	12.233	9.133	1.00	33.24
17127	C38	syr	F	1	12.266	11.866	9.655	1.00	36.47
17130	S39	syr	F	1	12.788	13.045	10.698	1.00	38.85
17131	O41	syr	F	1	12.756	14.346	9.987	1.00	40.15
17132	O40	syr	F	1	11.904	13.088	11.889	1.00	40.12



# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
17133	O42	syr	F	1	14.164	12.729	11.149	1.00	39.08
17134	C26	syr	F	1	7.068	6.175	11.112	1.00	15.95
17137	C25	syr	F	1	7.133	5.089	10.059	1.00	14.16
17140	C23	syr	F	1	7.708	3.745	10.538	1.00	12.85
17142	C24	syr	F	1	9.156	3.919	11.011	1.00	13.60
17146	C20	syr	F	1	6.808	3.066	11.583	1.00	12.50
17148	C21	syr	F	1	5.385	2.849	11.031	1.00	11.84
17151	C22	syr	F	1	4.890	1.506	11.583	1.00	12.25
17154	C14	syr	F	1	5.907	1.181	12.671	1.00	11.94
17156	C15	syr	F	1	7.225	1.672	12.086	1.00	12.32
17157	C19	syr	F	1	7.694	0.796	10.935	1.00	12.01
17161	C16	syr	F	1	8.236	1.632	13.241	1.00	11.77
17163	O18	syr	F	1	7.871	2.502	14.326	1.00	11.79
17165	C17	syr	F	1	8.405	0.195	13.756	1.00	11.59
17168	C12	syr	F	1	7.086	-0.504	14.184	1.00	11.97
17170	C2	syr	F	1	7.245	-2.008	14.515	1.00	12.39
17171	C8	syr	F	1	7.499	-2.832	13.245	1.00	13.73
17175	C1	syr	F	1	8.395	-2.319	15.496	1.00	11.40
17178	C6	syr	F	1	8.197	-1.721	16.898	1.00	11.99
17181	C5	syr	F	1	6.940	-2.338	17.503	1.00	12.62
17183	O7	syr	F	1	6.689	-1.854	18.826	1.00	13.11
17185	C4	syr	F	1	5.737	-2.016	16.614	1.00	11.66
17188	C3	syr	F	1	5.937	-2.499	15.172	1.00	12.17
17190	C9	syr	F	1	4.697	-2.131	14.333	1.00	12.07
17193	C10	syr	F	1	4.631	-0.662	13.868	1.00	11.38
17195	O13	syr	F	1	4.278	0.223	14.936	1.00	12.42
17197	C11	syr	F	1	5.943	-0.262	13.196	1.00	12.71
17199	O28	syr	F	2	-23.964	10.892	13.809	1.00	17.93
17200	C27	syr	F	2	-24.724	10.474	12.936	1.00	16.83
17201	N29	syr	F	2	-24.957	11.133	11.797	1.00	16.76
17203	C30	syr	F	2	-24.290	12.385	11.456	1.00	18.59
17206	C31	syr	F	2	-24.738	13.597	12.254	1.00	21.27
17209	C32	syr	F	2	-26.079	14.141	11.776	1.00	25.18
17212	N33	syr	F	2	-26.566	15.284	12.601	1.00	27.82
17213	C35	syr	F	2	-27.299	14.801	13.786	1.00	28.89
17217	C34	syr	F	2	-25.457	16.141	13.078	1.00	27.57
17221	C36	syr	F	2	-27.384	16.198	11.783	1.00	32.87
17224	C37	syr	F	2	-28.669	15.616	11.215	1.00	35.98
17227	C38	syr	F	2	-29.814	16.599	11.468	1.00	39.35
17230	S39	syr	F	2	-31.237	16.049	10.809	1.00	41.57
17231	O41	syr	F	2	-31.927	17.125	10.055	1.00	42.38
17232	O40	syr	F	2	-30.937	14.933	9.887	1.00	40.22
17233	O42	syr	F	2	-32.119	15.617	11.915	1.00	42.31
17234	C26	syr	F	2	-25.461	9.152	13.069	1.00	16.24
17237	C25	syr	F	2	-25.638	8.694	14.509	1.00	15.81
17240	C23	syr	F	2	-26.374	7.350	14.655	1.00	15.00
17242	C24	syr	F	2	-27.761	7.449	14.022	1.00	15.81
17246	C20	syr	F	2	-25.561	6.168	14.093	1.00	14.58
17248	C21	syr	F	2	-24.167	6.063	14.738	1.00	14.17

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
17251	C22	syr	F	2	-23.832	4.569	14.859	1.00	13.04
17254	C14	syr	F	2	-24.933	3.895	14.067	1.00	13.05
17256	C15	syr	F	2	-26.156	4.772	14.302	1.00	13.59
17257	C19	syr	F	2	-26.732	4.645	15.718	1.00	13.77
17261	C16	syr	F	2	-27.198	4.314	13.271	1.00	12.32
17263	O18	syr	F	2	-26.760	4.489	11.918	1.00	12.47
17265	C17	syr	F	2	-27.553	2.839	13.441	1.00	12.19
17268	C12	syr	F	2	-26.351	1.883	13.487	1.00	12.40
17270	C2	syr	F	2	-26.714	0.447	13.924	1.00	13.50
17271	C8	syr	F	2	-27.072	0.328	15.415	1.00	13.22
17275	C1	syr	F	2	-27.910	-0.134	13.153	1.00	12.64
17278	C6	syr	F	2	-27.695	-0.345	11.669	1.00	13.86
17281	C5	syr	F	2	-26.544	-1.309	11.459	1.00	12.95
17283	O7	syr	F	2	-26.312	-1.494	10.068	1.00	13.98
17285	C4	syr	F	2	-25.297	-0.731	12.137	1.00	13.06
17288	C3	syr	F	2	-25.512	-0.459	13.635	1.00	12.82
17290	C9	syr	F	2	-24.224	0.100	14.273	1.00	11.55
17293	C10	syr	F	2	-23.938	1.578	13.988	1.00	12.57
17295	O13	syr	F	2	-23.535	1.809	12.646	1.00	13.44
17297	C11	syr	F	2	-25.174	2.414	14.318	1.00	12.11
17299	O28	syr	F	3	-35.027	-44.086	-7.159	1.00	18.66
17300	C27	syr	F	3	-34.637	-43.565	-8.196	1.00	18.53
17301	N29	syr	F	3	-34.567	-44.217	-9.345	1.00	18.86
17303	C30	syr	F	3	-35.023	-45.580	-9.510	1.00	20.61
17306	C31	syr	F	3	-34.167	-46.618	-8.817	1.00	24.81
17309	C32	syr	F	3	-32.729	-46.534	-9.283	1.00	27.90
17312	N33	syr	F	3	-31.861	-47.547	-8.644	1.00	30.65
17313	C35	syr	F	3	-30.480	-47.280	-9.078	1.00	32.20
17317	C34	syr	F	3	-31.877	-47.379	-7.180	1.00	31.24
17321	C36	syr	F	3	-32.268	-48.931	-8.988	1.00	33.83
17324	C37	syr	F	3	-32.186	-49.194	-10.496	1.00	36.72
17327	C38	syr	F	3	-32.275	-50.679	-10.845	1.00	38.87
17330	S39	syr	F	3	-31.427	-50.998	-12.236	1.00	40.5
17331	O41	syr	F	3	-32.062	-50.435	-13.441	1.00	40.94
17332	O40	syr	F	3	-30.063	-50.431	-12.104	1.00	41.61
17333	O42	syr	F	3	-31.350	-52.480	-12.362	1.00	41.94
17334	C26	syr	F	3	-34.175	-42.121	-8.235	1.00	18.19
17337	C25	syr	F	3	-33.617	-41.682	-6.884	1.00	17.62
17340	C23	syr	F	3	-33.164	-40.214	-6.862	1.00	16.42
17342	C24	syr	F	3	-32.024	-40.019	-7.866	1.00	16.80
17346	C20	syr	F	3	-34.324	-39.211	-7.063	1.00	15.83
17348	C21	syr	F	3	-35.436	-39.434	-6.022	1.00	15.72
17351	C22	syr	F	3	-36.060	-38.061	-5.747	1.00	14.30
17354	C14	syr	F	3	-35.413	-37.148	-6.799	1.00	14.66
17356	C15	syr	F	3	-34.004	-37.719	-6.962	1.00	15.26
17357	C19	syr	F	3	-33.089	-37.470	-5.766	1.00	16.16
17361	C16	syr	F	3	-33.386	-37.058	-8.203	1.00	14.56
17363	O18	syr	F	3	-34.113	-37.354	-9.393	1.00	14.97
17365	C17	syr	F	3	-33.303	-35.535	-8.020	1.00	13.55

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
17368	C12	syr	F	3	-34.631	-34.861	-7.603	1.00	13.44
17370	C2	syr	F	3	-34.468	-33.389	-7.163	1.00	13.90
17371	C8	syr	F	3	-33.766	-33.276	-5.811	1.00	14.20
17375	C1	syr	F	3	-33.639	-32.547	-8.135	1.00	13.52
17378	C6	syr	F	3	-34.269	-32.376	-9.512	1.00	13.99
17381	C5	syr	F	3	-35.625	-31.697	-9.353	1.00	14.71
17383	O7	syr	F	3	-36.256	-31.564	-10.628	1.00	15.41
17385	C4	syr	F	3	-36.511	-32.528	-8.445	1.00	13.06
17388	C3	syr	F	3	-35.876	-32.772	-7.067	1.00	13.86
17390	C9	syr	F	3	-36.824	-33.601	-6.191	1.00	14.31
17393	C10	syr	F	3	-36.854	-35.106	-6.475	1.00	14.18
17395	O13	syr	F	3	-37.547	-35.433	-7.685	1.00	13.54
17397	C11	syr	F	3	-35.421	-35.648	-6.539	1.00	13.82
17399	O28	syr	F	4	-65.292	-47.138	-3.871	1.00	21.06
17400	C27	syr	F	4	-65.671	-47.252	-2.712	1.00	20.96
17401	N29	syr	F	4	-65.621	-48.398	-2.041	1.00	21.85
17403	C30	syr	F	4	-65.061	-49.627	-2.578	1.00	22.83
17406	C31	syr	F	4	-65.733	-50.202	-3.812	1.00	24.03
17409	C32	syr	F	4	-67.030	-50.931	-3.466	1.00	26.38
17412	N33	syr	F	4	-67.773	-51.435	-4.650	1.00	29.40
17413	C35	syr	F	4	-68.245	-50.294	-5.471	1.00	30.57
17417	C34	syr	F	4	-66.887	-52.244	-5.507	1.00	29.99
17421	C36	syr	F	4	-68.954	-52.208	-4.150	1.00	32.87
17424	C37	syr	F	4	-68.926	-53.751	-4.296	1.00	35.76
17427	C38	syr	F	4	-68.798	-54.547	-2.986	1.00	37.86
17430	S39	syr	F	4	-67.770	-55.858	-3.163	1.00	37.85
17431	O41	syr	F	4	-68.161	-56.657	-4.350	1.00	40.77
17432	O40	syr	F	4	-66.419	-55.309	-3.391	1.00	40.02
17433	O42	syr	F	4	-67.751	-56.734	-1.972	1.00	38.11
17434	C26	syr	F	4	-66.241	-46.076	-1.938	1.00	20.69
17437	C25	syr	F	4	-66.862	-45.032	-2.847	1.00	19.62
17440	C23	syr	F	4	-67.516	-43.858	-2.089	1.00	17.57
17442	C24	syr	F	4	-68.625	-44.376	-1.173	1.00	18.14
17446	C20	syr	F	4	-66.510	-42.984	-1.314	1.00	16.13
17448	C21	syr	F	4	-65.362	-42.473	-2.205	1.00	15.94
17451	C22	syr	F	4	-65.011	-41.062	-1.721	1.00	15.76
17454	C14	syr	F	4	-65.735	-40.939	-0.389	1.00	14.84
17456	C15	syr	F	4	-67.031	-41.699	-0.640	1.00	15.67
17457	C19	syr	F	4	-67.997	-40.958	-1.573	1.00	15.67
17461	C16	syr	F	4	-67.701	-41.852	0.735	1.00	14.79
17463	O18	syr	F	4	-66.926	-42.629	1.649	1.00	15.02
17465	C17	syr	F	4	-67.986	-40.482	1.374	1.00	15.41
17468	C12	syr	F	4	-66.767	-39.534	1.457	1.00	15.57
17470	C2	syr	F	4	-67.126	-38.085	1.874	1.00	17.08
17471	C8	syr	F	4	-67.871	-37.342	0.759	1.00	17.37
17475	C1	syr	F	4	-68.018	-38.029	3.120	1.00	17.48
17478	C6	syr	F	4	-67.351	-38.536	4.395	1.00	16.50
17481	C5	syr	F	4	-66.129	-37.685	4.703	1.00	16.69
17483	O7	syr	F	4	-65.494	-38.134	5.892	1.00	17.59

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
17485	C4	syr	F	4	-65.171	-37.767	3.523	1.00	16.35
17488	C3	syr	F	4	-65.815	-37.332	2.194	1.00	15.90
17490	C9	syr	F	4	-64.774	-37.450	1.061	1.00	15.43
17493	C10	syr	F	4	-64.563	-38.862	0.497	1.00	14.92
17495	O13	syr	F	4	-63.801	-39.667	1.388	1.00	15.44
17497	C11	syr	F	4	-65.909	-39.527	0.177	1.00	16.04
17499	O12	mes	G	1	12.814	1.616	7.937	1.00	24.67
17500	S9	mes	G	1	11.812	0.993	7.073	1.00	24.4
17501	O10	mes	G	1	12.046	1.445	5.675	1.00	27.22
17502	O11	mes	G	1	11.810	-0.461	7.171	1.00	28.23
17503	C8	mes	G	1	10.291	1.547	7.533	1.00	23.64
17506	C7	mes	G	1	9.219	0.851	6.686	1.00	24.05
17509	N1	mes	G	1	7.892	1.459	6.835	1.00	21.76
17510	C2	mes	G	1	7.792	2.837	6.370	1.00	21.74
17513	C3	mes	G	1	6.382	3.362	6.565	1.00	22.22
17516	O4	mes	G	1	5.463	2.466	5.939	1.00	22.65
17517	C5	mes	G	1	5.459	1.224	6.608	1.00	22.29
17520	C6	mes	G	1	6.805	0.535	6.449	1.00	22.27
17523	OW0	HOH	W	5	3.160	2.748	14.174	1.00	13.33
17526	OW0	HOH	W	6	-13.969	2.106	8.909	1.00	13.17
17529	OW0	HOH	W	7	2.400	-8.798	28.726	1.00	12.54
17532	OW0	HOH	W	8	-37.358	-27.466	-16.238	1.00	12.94
17535	OW0	HOH	W	9	-18.405	-5.556	8.958	1.00	13.40
17538	OW0	HOH	W	10	1.698	-11.209	30.000	1.00	12.33
17541	OW0	HOH	W	11	-1.765	-3.724	21.329	1.00	12.89
17544	OW0	HOH	W	12	-10.925	4.337	11.107	1.00	12.97
17547	OW0	HOH	W	13	-27.482	-5.272	4.368	1.00	12.44
17550	OW0	HOH	W	14	-23.304	-15.611	4.752	1.00	13.55
17553	OW0	HOH	W	15	-38.568	-38.052	-7.996	1.00	14.03
17556	OW0	HOH	W	16	-42.523	-21.035	-14.480	1.00	13.32
17559	OW0	HOH	W	17	-22.124	4.218	12.058	1.00	14.62
17562	OW0	HOH	W	18	-57.241	-34.684	6.393	1.00	16.43
17565	OW0	HOH	W	19	5.372	4.381	14.698	1.00	13.91
17568	OW0	HOH	W	20	7.429	-2.738	25.638	1.00	12.30
17571	OW0	HOH	W	21	-43.205	-18.306	-14.169	1.00	13.98
17574	OW0	HOH	W	22	-7.869	7.489	10.697	1.00	13.76
17577	OW0	HOH	W	23	-62.464	-41.940	0.277	1.00	16.16
17580	OW0	HOH	W	24	-37.601	-34.014	3.731	1.00	16.88
17583	OW0	HOH	W	25	-51.890	-44.165	-6.103	1.00	13.92
17586	OW0	HOH	W	26	-21.063	-0.277	23.661	1.00	16.52
17589	OW0	HOH	W	27	-23.585	-12.772	4.721	1.00	13.32
17592	OW0	HOH	W	28	-47.554	-37.579	-8.832	1.00	13.05
17595	OW0	HOH	W	29	-44.789	-29.284	-9.450	1.00	12.83
17598	OW0	HOH	W	30	-12.637	10.153	20.404	1.00	15.36
17601	OW0	HOH	W	31	-51.492	-41.734	-2.196	1.00	14.58
17604	OW0	HOH	W	32	-64.184	-43.953	1.149	1.00	16.01
17607	OW0	HOH	W	33	4.547	-12.698	20.606	1.00	15.39
17610	OW0	HOH	W	34	-57.593	-40.630	-13.633	1.00	15.06
17613	OW0	HOH	W	35	1.130	-6.405	6.065	1.00	14.70

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
17616	OW0	HOH	W	36	-44.196	-11.020	-32.107	1.00	16.83
17619	OW0	HOH	W	37	-7.703	11.012	15.980	1.00	14.52
17622	OW0	HOH	W	38	-36.691	-39.031	-9.765	1.00	15.37
17625	OW0	HOH	W	39	-8.515	10.307	13.378	1.00	15.27
17628	OW0	HOH	W	40	-33.690	-3.836	1.566	1.00	14.84
17631	OW0	HOH	W	42	-64.366	-32.426	-7.447	1.00	15.75
17634	OW0	HOH	W	43	13.829	-0.927	27.823	1.00	18.08
17637	OW0	HOH	W	44	6.013	-8.754	20.864	1.00	17.34
17640	OW0	HOH	W	45	0.034	-7.938	8.119	1.00	14.81
17643	OW0	HOH	W	46	-56.124	-42.529	-12.173	1.00	16.46
17646	OW0	HOH	W	47	-6.043	10.056	12.231	1.00	16.79
17649	OW0	HOH	W	48	0.481	-7.459	14.982	1.00	20.81
17652	OW0	HOH	W	49	-2.691	-12.024	44.776	1.00	18.21
17655	OW0	HOH	W	50	-5.049	3.623	17.688	1.00	13.00
17658	OW0	HOH	W	51	-50.211	-47.568	-1.329	1.00	16.60
17661	OW0	HOH	W	53	-43.072	-44.993	4.292	1.00	15.66
17664	OW0	HOH	W	54	-26.700	10.213	9.719	1.00	15.99
17667	OW0	HOH	W	55	-59.871	-28.162	16.222	1.00	18.10
17670	OW0	HOH	W	56	-44.477	-45.912	2.023	1.00	17.50
17673	OW0	HOH	W	57	-5.031	3.353	1.827	1.00	15.82
17676	OW0	HOH	W	58	-9.557	9.553	9.816	1.00	16.46
17679	OW0	HOH	W	59	-12.214	-9.995	32.224	1.00	16.98
17682	OW0	HOH	W	60	-33.711	-42.818	-11.633	1.00	17.75
17685	OW0	HOH	W	61	2.971	-13.013	16.601	1.00	17.88
17688	OW0	HOH	W	62	-24.105	5.720	10.859	1.00	14.78
17691	OW0	HOH	W	63	-39.094	-31.768	3.016	1.00	17.91
17694	OW0	HOH	W	64	-45.953	-17.126	-28.993	1.00	19.15
17697	OW0	HOH	W	65	1.078	-6.903	10.646	1.00	16.77
17700	OW0	HOH	W	66	-39.190	-18.915	-36.465	1.00	15.66
17703	OW0	HOH	W	68	-32.763	-4.589	7.887	1.00	14.84
17706	OW0	HOH	W	69	-10.435	8.327	13.391	1.00	14.30
17709	OW0	HOH	W	70	-48.632	-44.443	-4.209	1.00	15.61
17712	OW0	HOH	W	71	-49.471	-40.474	-6.170	1.00	14.81
17715	OW0	HOH	W	72	-60.414	-30.675	14.967	1.00	16.51
17718	OW0	HOH	W	73	-10.326	8.898	7.223	1.00	17.12
17721	OW0	HOH	W	74	-38.778	-31.366	0.016	1.00	17.73
17724	OW0	HOH	W	75	-48.121	-44.965	4.403	1.00	20.28
17727	OW0	HOH	W	76	-64.715	-37.547	12.805	1.00	17.42
17730	OW0	HOH	W	77	-70.865	-36.945	11.028	1.00	19.36
17733	OW0	HOH	W	78	-50.092	-45.041	-10.167	1.00	16.38
17736	OW0	HOH	W	80	-45.682	-29.714	0.480	1.00	20.84
17739	OW0	HOH	W	81	2.069	-13.959	20.830	1.00	16.49
17742	OW0	HOH	W	82	-11.231	-4.972	39.517	1.00	18.75
17745	OW0	HOH	W	83	-53.619	-40.960	1.536	1.00	14.31
17748	OW0	HOH	W	85	-46.180	-17.672	-37.651	1.00	16.50
17751	OW0	HOH	W	86	-31.272	-27.074	-14.177	1.00	18.33
17754	OW0	HOH	W	87	-8.473	0.005	43.758	1.00	18.40
17757	OW0	HOH	W	88	-13.536	9.392	23.022	1.00	15.07
17760	OW0	HOH	W	89	0.112	-18.225	30.231	1.00	18.19

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
17763	OWO	HOH	W	90	-23.583	-13.771	14.163	1.00	17.79
17766	OWO	HOH	W	91	-65.370	-27.386	7.899	1.00	20.87
17769	OWO	HOH	W	92	-51.641	-12.333	-31.122	1.00	18.48
17772	OWO	HOH	W	93	-21.369	-2.824	19.839	1.00	15.98
17775	OWO	HOH	W	94	8.538	8.289	13.576	1.00	15.84
17778	OWO	HOH	W	95	-41.132	-12.235	-25.581	1.00	20.50
17781	OWO	HOH	W	96	-50.176	-45.800	-7.498	1.00	16.80
17784	OWO	HOH	W	98	-57.325	-19.217	-12.226	1.00	20.77
17787	OWO	HOH	W	99	-7.816	5.006	14.536	1.00	12.96
17790	OWO	HOH	W	100	-42.141	-10.500	-18.556	1.00	17.48
17793	OWO	HOH	W	101	-5.772	5.441	3.729	1.00	16.47
17796	OWO	HOH	W	102	-10.228	-8.724	38.645	1.00	22.61
17799	OWO	HOH	W	103	-24.978	-15.995	-10.412	1.00	21.50
17802	OWO	HOH	W	104	-21.394	16.961	9.939	1.00	21.31
17805	OWO	HOH	W	105	-27.532	-22.625	0.523	1.00	22.49
17808	OWO	HOH	W	106	-26.005	-12.037	13.567	1.00	18.57
17811	OWO	HOH	W	107	11.706	-6.650	15.328	1.00	21.70
17814	OWO	HOH	W	108	-20.242	-2.818	22.587	1.00	16.60
17817	OWO	HOH	W	109	-28.573	9.826	6.943	1.00	18.24
17820	OWO	HOH	W	110	11.325	7.659	10.323	1.00	22.36
17823	OWO	HOH	W	111	-34.545	-30.119	-26.731	1.00	21.13
17826	OWO	HOH	W	112	-42.617	-14.503	-31.961	1.00	18.65
17829	OWO	HOH	W	113	10.930	8.997	12.657	1.00	22.28
17832	OWO	HOH	W	114	-63.082	-30.667	-5.649	1.00	18.00
17835	OWO	HOH	W	115	-22.743	-22.048	7.803	1.00	20.68
17838	OWO	HOH	W	116	4.457	-16.096	37.151	1.00	16.12
17841	OWO	HOH	W	117	-32.860	-42.024	-14.942	1.00	20.21
17844	OWO	HOH	W	118	-58.009	-22.186	-27.714	1.00	19.46
17847	OWO	HOH	W	119	-43.766	-12.258	-10.477	1.00	21.92
17850	OWO	HOH	W	120	-29.928	-10.195	11.073	1.00	21.48
17853	OWO	HOH	W	121	8.328	-5.870	46.552	1.00	23.04
17856	OWO	HOH	W	122	-63.237	-32.105	-2.842	1.00	18.35
17859	OWO	HOH	W	123	-24.453	-10.640	17.289	1.00	19.63
17862	OWO	HOH	W	124	-11.855	10.278	11.043	1.00	19.82
17865	OWO	HOH	W	125	3.974	-4.952	43.680	1.00	21.74
17868	OWO	HOH	W	126	-32.221	-12.635	6.619	1.00	18.49
17871	OWO	HOH	W	127	16.248	5.924	26.336	1.00	20.89
17874	OWO	HOH	W	128	-43.965	-31.668	21.694	1.00	22.99
17877	OWO	HOH	W	129	-29.338	-20.457	-5.946	1.00	23.65
17880	OWO	HOH	W	130	-32.201	-3.617	15.068	1.00	19.54
17883	OWO	HOH	W	131	12.619	-4.375	22.440	1.00	15.51
17886	OWO	HOH	W	132	-45.517	-23.821	-38.055	1.00	21.98
17889	OWO	HOH	W	133	-50.132	-46.854	-3.986	1.00	17.33
17892	OWO	HOH	W	134	-56.817	-15.729	-16.504	1.00	21.47
17895	OWO	HOH	W	135	8.300	-17.983	31.664	1.00	22.83
17898	OWO	HOH	W	136	-43.716	-40.739	-24.290	1.00	20.75
17901	OWO	HOH	W	137	-38.034	-23.401	-2.461	1.00	20.21
17904	OWO	HOH	W	138	-37.332	-21.541	-6.805	1.00	18.87
17907	OWO	HOH	W	139	-58.779	-42.194	-15.558	1.00	22.26

## FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
17910	OW0	HOH	W	140	-10.168	-16.467	-6.034	1.00	22.30
17913	OW0	HOH	W	141	10.231	9.126	16.325	1.00	16.79
17916	OW0	HOH	W	142	-19.548	10.710	17.395	1.00	18.70
17919	OW0	HOH	W	143	-9.676	3.650	3.058	1.00	18.79
17922	OW0	HOH	W	144	-53.281	-43.836	-21.712	1.00	24.79
17925	OW0	HOH	W	145	-31.959	-27.404	-20.679	1.00	20.78
17928	OW0	HOH	W	146	-26.836	-8.447	11.395	1.00	20.34
17931	OW0	HOH	W	147	13.038	4.377	32.227	1.00	21.64
17934	OW0	HOH	W	148	-20.999	-5.517	16.212	1.00	20.13
17937	OW0	HOH	W	149	4.525	-17.506	30.244	1.00	22.79
17940	OW0	HOH	W	150	-32.280	-1.357	-4.997	1.00	20.46
17943	OW0	HOH	W	151	-27.192	-4.926	13.638	1.00	27.01
17946	OW0	HOH	W	152	-56.571	-29.518	-2.109	1.00	22.13
17949	OW0	HOH	W	153	-62.513	-19.851	-5.792	1.00	20.88
17952	OW0	HOH	W	154	-37.414	-50.613	-10.474	1.00	20.20
17955	OW0	HOH	W	155	-40.510	-12.696	-28.519	1.00	23.01
17958	OW0	HOH	W	156	2.830	13.344	27.970	1.00	24.67
17961	OW0	HOH	W	157	7.472	-6.985	19.672	1.00	22.18
17964	OW0	HOH	W	158	-31.050	-12.055	-22.699	1.00	30.38
17967	OW0	HOH	W	159	-47.426	-45.956	-7.043	1.00	21.22
17970	OW0	HOH	W	160	17.043	-5.640	43.857	1.00	21.26
17973	OW0	HOH	W	161	-32.980	-12.370	-15.457	1.00	19.37
17976	OW0	HOH	W	162	8.777	-10.500	22.312	1.00	20.59
17979	OW0	HOH	W	163	1.368	6.276	6.136	1.00	21.51
17982	OW0	HOH	W	164	-8.847	8.324	21.899	1.00	21.51
17985	OW0	HOH	W	165	-5.534	-7.933	13.137	1.00	25.03
17988	OW0	HOH	W	166	-13.160	-1.120	-5.473	1.00	23.89
17991	OW0	HOH	W	167	-42.866	-10.327	-21.238	1.00	22.56
17994	OW0	HOH	W	168	-46.700	-52.498	9.243	1.00	24.38
17997	OW0	HOH	W	169	-45.887	-26.385	14.787	1.00	21.29
18000	OW0	HOH	W	170	-3.690	4.666	-0.190	1.00	22.34
18003	OW0	HOH	W	171	-9.547	-17.730	2.636	1.00	20.70
18006	OW0	HOH	W	172	1.010	-18.305	32.901	1.00	21.57
18009	OW0	HOH	W	173	-27.658	13.678	8.549	1.00	28.50
18012	OW0	HOH	W	174	-33.836	-15.532	-33.204	1.00	25.82
18015	OW0	HOH	W	176	-9.282	6.051	12.485	1.00	11.86
18018	OW0	HOH	W	177	-50.367	-42.439	-4.579	1.00	12.26
18021	OW0	HOH	W	178	11.319	-11.950	41.315	1.00	17.07
18024	OW0	HOH	W	179	-10.506	-8.799	41.179	1.00	22.68
18027	OW0	HOH	W	180	-12.190	-13.758	-12.289	1.00	20.41
18030	OW0	HOH	W	181	-53.158	-10.739	-18.312	1.00	21.04
18033	OW0	HOH	W	182	-39.554	-20.344	-5.592	1.00	23.14
18036	OW0	HOH	W	183	-58.831	-19.886	-21.059	1.00	19.42
18039	OW0	HOH	W	184	-39.845	-9.165	-18.036	1.00	25.77
18042	OW0	HOH	W	185	10.813	-10.921	27.404	1.00	18.53
18045	OW0	HOH	W	186	-41.730	-47.115	5.086	1.00	24.01
18048	OW0	HOH	W	187	-61.917	-44.966	-7.946	1.00	20.01
18051	OW0	HOH	W	188	-19.906	1.432	29.536	1.00	21.88
18054	OW0	HOH	W	189	4.912	-14.789	39.537	1.00	20.92

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
18057	OWO	HOH	W	190	-50.340	-53.076	-9.985	1.00	26.60
18060	OWO	HOH	W	191	-9.417	-18.952	-6.826	1.00	23.96
18063	OWO	HOH	W	192	-38.372	-44.937	-2.609	1.00	21.01
18066	OWO	HOH	W	193	-56.644	-52.391	12.783	1.00	26.23
18069	OWO	HOH	W	194	-7.154	-17.926	-2.156	1.00	23.68
18072	OWO	HOH	W	195	-66.717	-48.488	0.619	1.00	20.03
18075	OWO	HOH	W	196	-29.930	-33.875	-23.417	1.00	22.67
18078	OWO	HOH	W	197	-48.549	-15.955	-31.943	1.00	24.95
18081	OWO	HOH	W	198	-24.108	16.539	9.776	1.00	22.27
18084	OWO	HOH	W	199	-62.999	-28.125	-14.418	1.00	25.08
18087	OWO	HOH	W	200	-3.601	-18.614	7.961	1.00	22.46
18090	OWO	HOH	W	201	-44.438	-37.268	26.089	1.00	22.26
18093	OWO	HOH	W	202	0.532	14.738	23.517	1.00	22.34
18096	OWO	HOH	W	203	-62.081	-22.916	-15.715	1.00	22.40
18099	OWO	HOH	W	204	-5.135	-14.543	-1.823	1.00	24.53
18102	OWO	HOH	W	205	-64.980	-26.647	3.537	1.00	23.24
18105	OWO	HOH	W	206	4.386	14.879	9.762	1.00	24.03
18108	OWO	HOH	W	207	-48.813	-12.030	-31.633	1.00	25.78
18111	OWO	HOH	W	208	-9.966	-10.165	17.887	1.00	31.47
18114	OWO	HOH	W	209	-10.102	11.048	20.429	1.00	26.61
18117	OWO	HOH	W	210	6.918	14.306	21.078	1.00	22.67
18120	OWO	HOH	W	211	-62.437	-45.019	-14.011	1.00	26.58
18123	OWO	HOH	W	212	-2.958	0.686	8.008	1.00	25.75
18126	OWO	HOH	W	213	-65.845	-31.471	8.155	1.00	26.66
18129	OWO	HOH	W	214	-38.253	-29.441	4.645	1.00	25.37
18132	OWO	HOH	W	215	-52.645	-40.045	-13.399	1.00	23.21
18135	OWO	HOH	W	216	-55.337	-53.220	7.911	1.00	25.74
18138	OWO	HOH	W	217	-52.753	-47.064	-4.508	1.00	21.80
18141	OWO	HOH	W	218	-10.575	-10.994	37.163	1.00	24.60
18144	OWO	HOH	W	219	-26.456	-9.153	-18.769	1.00	24.83
18147	OWO	HOH	W	220	-35.430	7.438	3.711	1.00	25.73
18150	OWO	HOH	W	221	-31.225	-17.601	-14.486	1.00	33.18
18153	OWO	HOH	W	222	-67.567	-49.660	3.741	1.00	21.92
18156	OWO	HOH	W	223	-14.412	11.680	24.092	1.00	22.22
18159	OWO	HOH	W	224	-29.657	-28.389	-7.131	1.00	25.41
18162	OWO	HOH	W	225	-63.190	-25.352	7.516	1.00	20.99
18165	OWO	HOH	W	226	-53.596	-24.293	-33.203	1.00	23.55
18168	OWO	HOH	W	227	-8.459	16.641	7.054	1.00	27.01
18171	OWO	HOH	W	229	-8.567	-9.165	43.067	1.00	23.21
18174	OWO	HOH	W	230	-3.649	0.152	-4.673	1.00	23.80
18177	OWO	HOH	W	231	-69.845	-40.672	16.319	1.00	23.89
18180	OWO	HOH	W	232	-9.793	14.825	17.468	1.00	27.77
18183	OWO	HOH	W	233	19.188	4.350	4.555	1.00	26.21
18186	OWO	HOH	W	234	-5.748	12.057	10.445	1.00	26.02
18189	OWO	HOH	W	235	-45.888	-28.184	21.431	1.00	25.39
18192	OWO	HOH	W	236	12.533	-0.637	46.753	1.00	25.86
18195	OWO	HOH	W	237	-35.957	-9.155	-23.033	1.00	22.15
18198	OWO	HOH	W	238	-71.080	-47.817	15.103	1.00	26.65
18201	OWO	HOH	W	240	-10.340	7.705	-4.987	1.00	25.15



# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
18204	OW0	HOH	W	241	-30.388	-17.475	-27.757	1.00	27.53
18207	OW0	HOH	W	242	-29.344	-31.938	-2.430	1.00	26.91
18210	OW0	HOH	W	243	-59.487	-46.574	-14.831	1.00	26.42
18213	OW0	HOH	W	244	-40.639	-50.126	2.221	1.00	28.73
18216	OW0	HOH	W	245	-45.408	-13.753	-32.846	1.00	25.99
18219	OW0	HOH	W	246	-58.768	-18.983	6.313	1.00	25.71
18222	OW0	HOH	W	247	-32.618	-20.058	-12.199	1.00	24.98
18225	OW0	HOH	W	248	-2.580	-9.550	-0.531	1.00	24.03
18228	OW0	HOH	W	249	-51.020	-16.853	-33.405	1.00	26.40
18231	OW0	HOH	W	250	-12.041	8.554	-2.460	1.00	28.29
18234	OW0	HOH	W	251	-57.305	-17.080	-18.906	1.00	25.77
18237	OW0	HOH	W	252	7.156	-8.694	2.222	1.00	25.66
18240	OW0	HOH	W	253	-23.758	-23.212	5.347	1.00	25.40
18243	OW0	HOH	W	254	-36.798	4.629	14.730	1.00	28.30
18246	OW0	HOH	W	255	-6.432	-14.579	40.123	1.00	25.01
18249	OW0	HOH	W	256	-2.342	3.418	-2.175	1.00	26.65
18252	OW0	HOH	W	257	-53.778	-10.106	-20.902	1.00	26.07
18255	OW0	HOH	W	258	13.288	-7.236	21.507	1.00	28.59
18258	OW0	HOH	W	259	-61.725	-31.466	1.366	1.00	21.28
18261	OW0	HOH	W	260	-13.012	10.068	7.456	1.00	26.12
18264	OW0	HOH	W	261	-59.143	-36.100	-19.615	1.00	26.51
18267	OW0	HOH	W	262	-27.803	-6.209	11.652	1.00	25.18
18270	OW0	HOH	W	263	-48.955	-51.868	7.139	1.00	29.29
18273	OW0	HOH	W	264	-40.489	-28.830	-3.248	1.00	19.64
18276	OW0	HOH	W	265	-63.723	-23.828	-18.161	1.00	25.99
18279	OW0	HOH	W	266	-46.457	-25.970	20.142	1.00	25.17
18282	OW0	HOH	W	267	-51.201	-44.238	-19.699	1.00	26.14
18285	OW0	HOH	W	270	-64.581	-22.626	-23.955	1.00	24.82
18288	OW0	HOH	W	271	-8.518	-18.957	0.220	1.00	25.72
18291	OW0	HOH	W	272	-4.903	-14.971	-10.304	1.00	27.69
18294	OW0	HOH	W	273	-37.605	-29.451	7.487	1.00	36.34
18297	OW0	HOH	W	274	-37.905	-11.916	-28.841	1.00	20.81
18300	OW0	HOH	W	275	-29.480	-17.850	-12.399	1.00	24.35
18303	OW0	HOH	W	276	-30.877	-0.503	19.834	1.00	24.80
18306	OW0	HOH	W	277	-38.746	-23.236	0.132	1.00	30.94
18309	OW0	HOH	W	278	7.042	14.153	10.235	1.00	24.33
18312	OW0	HOH	W	279	-36.480	-0.333	5.176	1.00	20.24
18315	OW0	HOH	W	280	15.884	-8.312	44.333	1.00	28.11
18318	OW0	HOH	W	281	-0.297	-7.890	0.232	1.00	22.17
18321	OW0	HOH	W	282	-35.486	-11.067	1.523	1.00	26.97
18324	OW0	HOH	W	283	-45.926	-20.885	7.139	1.00	44.84
18327	OW0	HOH	W	284	-61.977	-29.018	29.362	1.00	37.50
18330	OW0	HOH	W	285	-15.903	-4.472	34.600	1.00	22.26
18333	OW0	HOH	W	286	-20.812	6.999	-5.144	1.00	24.21
18336	OW0	HOH	W	287	-31.491	-14.815	-16.242	1.00	23.70
18339	OW0	HOH	W	288	-72.368	-34.371	4.276	1.00	24.47
18342	OW0	HOH	W	289	-53.540	-56.120	-3.123	1.00	27.28
18345	OW0	HOH	W	290	-30.004	-25.072	-12.494	1.00	28.70
18348	OW0	HOH	W	291	-35.002	-49.562	-11.116	1.00	22.24

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
18351	OWO	HOH	W	293	-33.549	-11.608	8.795	1.00	28.82
18354	OWO	HOH	W	294	14.452	-7.776	31.115	1.00	27.58
18357	OWO	HOH	W	295	-72.431	-34.473	10.610	1.00	29.40
18360	OWO	HOH	W	296	-21.031	-5.168	24.116	1.00	28.11
18363	OWO	HOH	W	297	-31.863	-13.045	10.726	1.00	26.59
18366	OWO	HOH	W	298	10.320	-13.084	23.899	1.00	26.77
18369	OWO	HOH	W	299	-12.808	8.161	30.529	1.00	24.26
18372	OWO	HOH	W	300	-2.914	18.689	12.738	1.00	23.60
18375	OWO	HOH	W	301	-18.270	9.802	-1.767	1.00	25.62
18378	OWO	HOH	W	302	-7.258	15.618	27.123	1.00	27.73
18381	OWO	HOH	W	303	-25.489	12.395	15.797	1.00	27.05
18384	OWO	HOH	W	304	-48.865	-54.255	-5.589	1.00	30.51
18387	OWO	HOH	W	305	1.047	-10.349	7.561	1.00	27.50
18390	OWO	HOH	W	306	7.856	-21.381	34.620	1.00	30.83
18393	OWO	HOH	W	307	-48.471	-45.315	14.846	1.00	30.20
18396	OWO	HOH	W	308	-44.675	-44.143	-20.716	1.00	23.88
18399	OWO	HOH	W	309	-62.027	-54.153	-4.459	1.00	26.43
18402	OWO	HOH	W	310	-3.815	-17.516	15.090	1.00	27.30
18405	OWO	HOH	W	311	-53.048	-19.556	9.947	1.00	29.57
18408	OWO	HOH	W	312	10.753	-6.514	10.479	1.00	34.78
18411	OWO	HOH	W	313	-36.380	3.671	1.448	1.00	28.05
18414	OWO	HOH	W	314	-1.661	-20.037	29.246	1.00	26.80
18417	OWO	HOH	W	316	-33.945	-40.059	-1.106	1.00	38.52
18420	OWO	HOH	W	317	-5.759	14.790	24.690	1.00	27.42
18423	OWO	HOH	W	318	-63.951	-45.304	-9.634	1.00	23.44
18426	OWO	HOH	W	319	-40.575	-31.029	15.729	1.00	26.40
18429	OWO	HOH	W	320	0.844	-17.443	23.281	1.00	31.23
18432	OWO	HOH	W	321	-47.105	-45.700	-10.135	1.00	25.74
18435	OWO	HOH	W	322	-30.540	-32.946	6.342	1.00	33.75
18438	OWO	HOH	W	323	13.846	-10.878	40.681	1.00	20.78
18441	OWO	HOH	W	324	-36.933	-36.044	9.625	1.00	23.21
18444	OWO	HOH	W	325	-52.809	-48.610	-1.298	1.00	26.95
18447	OWO	HOH	W	326	-56.879	-35.192	29.412	1.00	25.90
18450	OWO	HOH	W	328	-4.706	11.224	14.521	1.00	22.53
18453	OWO	HOH	W	329	-15.033	-5.938	18.283	1.00	26.89
18456	OWO	HOH	W	330	-8.118	6.992	3.457	1.00	29.08
18459	OWO	HOH	W	331	-11.360	-14.453	30.730	1.00	30.22
18462	OWO	HOH	W	332	-40.563	-23.004	8.766	1.00	28.63
18465	OWO	HOH	W	333	-4.570	-18.722	4.095	1.00	24.32
18468	OWO	HOH	W	334	-27.198	-20.743	7.367	1.00	29.55
18471	OWO	HOH	W	335	-36.570	-24.752	-8.857	1.00	27.52
18474	OWO	HOH	W	336	-4.406	-17.300	-2.295	1.00	29.36
18477	OWO	HOH	W	337	-26.968	-0.641	28.021	1.00	31.99
18480	OWO	HOH	W	338	-5.803	7.574	31.791	1.00	24.96
18483	OWO	HOH	W	339	-37.901	-44.366	-20.377	1.00	26.69
18486	OWO	HOH	W	340	2.788	-14.073	9.565	1.00	28.44
18489	OWO	HOH	W	342	5.291	-11.336	2.718	1.00	29.33
18492	OWO	HOH	W	343	0.056	-17.754	4.264	1.00	29.73
18495	OWO	HOH	W	344	-5.980	-0.954	-4.530	1.00	23.30

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
18498	OW0	HOH	W	345	-29.003	11.548	9.368	1.00	26.80
18501	OW0	HOH	W	346	-23.132	-10.904	19.761	1.00	35.51
18504	OW0	HOH	W	347	-1.407	-9.845	-3.107	1.00	30.69
18507	OW0	HOH	W	348	-53.798	-49.517	-5.461	1.00	37.45
18510	OW0	HOH	W	349	-13.686	-1.143	-12.337	1.00	32.42
18513	OW0	HOH	W	350	-13.580	17.339	5.484	1.00	24.55
18516	OW0	HOH	W	351	13.903	-9.607	43.225	1.00	23.19
18519	OW0	HOH	W	352	-60.262	-17.580	-21.781	1.00	25.69
18522	OW0	HOH	W	353	-52.844	-55.809	-13.467	1.00	28.53
18525	OW0	HOH	W	354	-6.591	-13.605	42.723	1.00	25.11
18528	OW0	HOH	W	355	-8.506	17.798	11.713	1.00	24.54
18531	OW0	HOH	W	356	-3.830	-13.879	-4.200	1.00	26.92
18534	OW0	HOH	W	357	-11.681	-20.350	-5.993	1.00	27.86
18537	OW0	HOH	W	358	12.774	-2.705	48.606	1.00	32.76
18540	OW0	HOH	W	359	-44.938	-28.225	23.890	1.00	26.70
18543	OW0	HOH	W	360	-56.969	-14.034	-29.181	1.00	25.04
18546	OW0	HOH	W	362	-66.900	-45.851	20.144	1.00	28.35
18549	OW0	HOH	W	363	-37.469	-0.629	18.071	1.00	32.58
18552	OW0	HOH	W	364	-21.322	-5.735	27.240	1.00	35.64
18555	OW0	HOH	W	365	-2.703	-7.322	-10.898	1.00	28.00
18558	OW0	HOH	W	366	6.561	-19.125	33.881	1.00	28.24
18561	OW0	HOH	W	367	-3.303	-18.148	-4.554	1.00	25.16
18564	OW0	HOH	W	368	-33.725	-6.458	9.912	1.00	29.75
18567	OW0	HOH	W	369	-16.850	6.238	39.214	1.00	32.73
18570	OW0	HOH	W	370	-59.715	-39.584	-5.559	1.00	28.64
18573	OW0	HOH	W	371	-61.575	-24.026	24.172	1.00	28.92
18576	OW0	HOH	W	372	-37.037	-31.854	-31.885	1.00	31.51
18579	OW0	HOH	W	373	-9.915	-2.000	45.285	1.00	24.74
18582	OW0	HOH	W	374	-36.231	-12.027	-33.152	1.00	27.77
18585	OW0	HOH	W	375	-13.395	-6.811	-13.569	1.00	32.62
18588	OW0	HOH	W	376	-42.877	-29.923	23.593	1.00	30.90
18591	OW0	HOH	W	377	-60.773	-41.179	-16.925	1.00	28.65
18594	OW0	HOH	W	378	-20.937	11.984	19.253	1.00	25.02
18597	OW0	HOH	W	379	-12.290	-6.568	41.405	1.00	27.25
18600	OW0	HOH	W	380	-64.538	-53.812	-3.383	1.00	23.47
18603	OW0	HOH	W	381	-35.694	-12.611	-30.298	1.00	30.62
18606	OW0	HOH	W	383	9.818	11.435	12.764	1.00	24.30
18609	OW0	HOH	W	385	-8.769	9.525	5.220	1.00	28.62
18612	OW0	HOH	W	386	-62.118	-53.986	7.261	1.00	27.18
18615	OW0	HOH	W	387	3.706	-6.504	10.132	1.00	27.74
18618	OW0	HOH	W	388	-37.714	-48.162	2.304	1.00	30.25
18621	OW0	HOH	W	389	-13.036	-13.429	28.981	1.00	29.51
18624	OW0	HOH	W	390	-41.283	-39.436	-1.810	1.00	28.81
18627	OW0	HOH	W	391	-62.301	-25.071	-13.762	1.00	24.83
18630	OW0	HOH	W	392	-31.210	-15.600	9.701	1.00	28.85
18633	OW0	HOH	W	393	-6.075	-16.250	21.654	1.00	28.42
18636	OW0	HOH	W	394	-46.551	-9.866	-23.520	1.00	33.59
18639	OW0	HOH	W	395	-37.774	-8.946	-26.992	1.00	33.88
18642	OW0	HOH	W	397	-15.081	9.649	30.184	1.00	23.30

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
18645	OWO	HOH	W	398	16.972	-13.730	34.822	1.00	28.64
18648	OWO	HOH	W	399	-44.271	-53.547	-9.591	1.00	29.37
18651	OWO	HOH	W	400	16.945	-3.915	45.956	1.00	34.07
18654	OWO	HOH	W	401	10.941	18.797	15.634	1.00	31.38
18657	OWO	HOH	W	402	-36.405	-45.691	-1.181	1.00	24.16
18660	OWO	HOH	W	403	-10.684	19.073	18.741	1.00	27.95
18663	OWO	HOH	W	404	-15.947	-0.760	42.197	1.00	27.69
18666	OWO	HOH	W	405	-39.088	-34.392	11.658	1.00	30.88
18669	OWO	HOH	W	407	-22.298	-5.753	14.299	1.00	30.26
18672	OWO	HOH	W	408	2.062	-11.300	-0.597	1.00	36.53
18675	OWO	HOH	W	409	-1.286	-19.062	34.575	1.00	33.94
18678	OWO	HOH	W	410	-11.028	-20.623	5.831	1.00	32.87
18681	OWO	HOH	W	411	-15.819	11.553	26.533	1.00	29.12
18684	OWO	HOH	W	412	-30.509	-16.904	-30.347	1.00	43.18
18687	OWO	HOH	W	413	-54.968	-56.305	-10.204	1.00	30.99
18690	OWO	HOH	W	414	-25.437	-17.724	13.728	1.00	33.57
18693	OWO	HOH	W	415	-2.654	17.495	9.330	1.00	27.17
18696	OWO	HOH	W	416	-17.049	-2.680	36.519	1.00	28.71
18699	OWO	HOH	W	417	-15.673	15.186	21.499	1.00	30.76
18702	OWO	HOH	W	418	-15.874	9.857	32.745	1.00	33.08
18705	OWO	HOH	W	420	-26.421	-12.501	17.570	1.00	30.34
18708	OWO	HOH	W	421	1.504	-14.079	14.635	1.00	30.61
18711	OWO	HOH	W	422	-56.500	-15.066	-23.319	1.00	29.79
18714	OWO	HOH	W	423	-16.530	-24.545	-2.193	1.00	29.50
18717	OWO	HOH	W	424	-12.731	12.937	10.897	1.00	39.31
18720	OWO	HOH	W	426	-6.094	-18.915	13.035	1.00	32.52
18723	OWO	HOH	W	428	-32.941	-50.902	-18.961	1.00	32.99
18726	OWO	HOH	W	429	-44.113	-26.160	16.852	1.00	31.24
18729	OWO	HOH	W	430	-11.752	-19.209	-3.613	1.00	25.94
18732	OWO	HOH	W	431	-33.162	-44.863	-5.298	1.00	28.90
18735	OWO	HOH	W	433	-45.084	-11.201	-8.280	1.00	34.55
18738	OWO	HOH	W	434	-2.717	3.699	46.035	1.00	29.96
18741	OWO	HOH	W	436	-44.025	-20.308	2.812	1.00	31.50
18744	OWO	HOH	W	438	-14.537	-7.673	36.525	1.00	30.71
18747	OWO	HOH	W	439	-7.539	-19.609	-4.534	1.00	26.39
18750	OWO	HOH	W	440	-2.634	8.620	0.399	1.00	31.25
18753	OWO	HOH	W	441	-8.302	-17.813	25.727	1.00	31.43
18756	OWO	HOH	W	442	-33.455	-30.698	-28.963	1.00	41.91
18759	OWO	HOH	W	444	-49.699	-46.855	-13.558	1.00	31.32
18762	OWO	HOH	W	445	-39.672	-13.469	-9.710	1.00	26.08
18765	OWO	HOH	W	446	-16.058	4.331	18.700	1.00	34.03
18768	OWO	HOH	W	447	-17.671	-0.707	31.115	1.00	27.75
18771	OWO	HOH	W	448	-10.700	12.310	33.920	1.00	38.15
18774	OWO	HOH	W	449	-19.100	8.775	-4.201	1.00	28.23
18777	OWO	HOH	W	450	-72.598	-34.907	-1.489	1.00	27.54
18780	OWO	HOH	W	451	-37.910	-34.806	22.808	1.00	29.80
18783	OWO	HOH	W	452	-50.596	-23.185	24.234	1.00	28.13
18786	OWO	HOH	W	453	-39.841	-45.218	10.659	1.00	29.59
18789	OWO	HOH	W	454	-45.509	-52.769	-12.965	1.00	25.19

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
18792	OW0	HOH	W	455	-26.257	-20.190	9.877	1.00	33.71
18795	OW0	HOH	W	458	-13.799	-20.923	-7.681	1.00	31.12
18798	OW0	HOH	W	459	9.418	-9.040	44.613	1.00	31.24
18801	OW0	HOH	W	460	-39.700	-46.915	6.860	1.00	30.19
18804	OW0	HOH	W	461	-55.979	-28.739	-29.600	1.00	29.08
18807	OW0	HOH	W	462	-65.033	-31.061	-13.532	1.00	23.41
18810	OW0	HOH	W	465	-31.048	-26.571	-29.971	1.00	29.32
18813	OW0	HOH	W	466	-36.654	-3.577	-1.152	1.00	33.65
18816	OW0	HOH	W	467	-45.535	-9.373	-21.146	1.00	35.79
18819	OW0	HOH	W	468	0.609	-7.757	-2.459	1.00	29.63
18822	OW0	HOH	W	469	-16.451	-3.277	32.122	1.00	32.88
18825	OW0	HOH	W	470	-2.735	-6.841	49.722	1.00	29.17
18828	OW0	HOH	W	471	-65.338	-30.636	-24.548	1.00	31.25
18831	OW0	HOH	W	472	-19.088	0.637	33.378	1.00	33.25
18834	OW0	HOH	W	473	-50.633	-29.798	-36.139	1.00	31.11
18837	OW0	HOH	W	474	9.192	-14.753	26.000	1.00	25.07
18840	OW0	HOH	W	475	17.018	0.044	30.109	1.00	36.34
18843	OW0	HOH	W	476	-24.949	-5.044	19.888	1.00	36.18
18846	OW0	HOH	W	477	-54.507	-53.813	13.818	1.00	31.64
18849	OW0	HOH	W	478	-30.091	-0.006	-11.086	1.00	35.00
18852	OW0	HOH	W	482	-20.610	2.641	31.813	1.00	37.42
18855	OW0	HOH	W	484	-25.532	-23.597	2.282	1.00	30.71
18858	OW0	HOH	W	486	-64.609	-22.399	10.458	1.00	31.67
18861	OW0	HOH	W	487	16.932	-0.067	22.891	1.00	30.57
18864	OW0	HOH	W	488	-58.168	-15.758	-21.081	1.00	30.20
18867	OW0	HOH	W	489	-46.600	-48.543	-7.085	1.00	33.74
18870	OW0	HOH	W	490	-54.317	-50.893	-15.774	1.00	29.36
18873	OW0	HOH	W	491	-57.157	-16.380	14.173	1.00	32.16
18876	OW0	HOH	W	492	2.345	-17.230	36.277	1.00	31.13
18879	OW0	HOH	W	493	-32.419	-45.859	-12.912	1.00	27.08
18882	OW0	HOH	W	494	-27.687	-22.639	-2.233	1.00	28.05
18885	OW0	HOH	W	497	-50.273	-48.879	-15.412	1.00	46.28
18888	OW0	HOH	W	498	-56.600	-21.350	-32.027	1.00	40.63
18891	OW0	HOH	W	499	-13.718	18.047	8.906	1.00	30.27
18894	OW0	HOH	W	500	-48.141	-49.051	-0.489	1.00	33.22
18897	OW0	HOH	W	501	-34.398	-20.239	-5.962	1.00	26.31
18900	OW0	HOH	W	502	-59.702	-21.121	16.655	1.00	31.19
18903	OW0	HOH	W	503	-27.477	18.555	2.591	1.00	31.48
18906	OW0	HOH	W	504	-49.875	-24.271	26.689	1.00	33.41
18909	OW0	HOH	W	505	-16.546	-10.860	30.920	1.00	39.53
18912	OW0	HOH	W	506	-45.696	-41.578	-25.946	1.00	29.86
18915	OW0	HOH	W	507	-63.436	-41.314	34.375	1.00	35.31
18918	OW0	HOH	W	508	-52.733	-32.974	-27.462	1.00	35.28
18921	OW0	HOH	W	509	-50.079	-51.017	0.775	1.00	29.75
18924	OW0	HOH	W	510	-27.821	-27.489	-21.645	1.00	36.47
18927	OW0	HOH	W	511	-13.516	-9.972	34.666	1.00	32.67
18930	OW0	HOH	W	512	-20.209	11.160	26.051	1.00	30.90
18933	OW0	HOH	W	513	-11.062	10.738	3.843	1.00	28.99
18936	OW0	HOH	W	515	6.418	5.033	47.899	1.00	28.62

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
18939	OW0	HOH	W	516	-49.687	-19.874	-37.460	1.00	36.05
18942	OW0	HOH	W	517	-65.701	-19.157	-9.131	1.00	38.40
18945	OW0	HOH	W	518	-57.640	-18.264	-9.917	1.00	37.06
18948	OW0	HOH	W	519	2.486	16.054	21.565	1.00	32.08
18951	OW0	HOH	W	520	-59.185	-18.089	-13.748	1.00	37.57
18954	OW0	HOH	W	521	-39.347	-9.282	-15.415	1.00	28.47
18957	OW0	HOH	W	523	-67.566	-51.893	-0.108	1.00	31.71
18960	OW0	HOH	W	524	-2.061	16.586	6.336	1.00	35.98
18963	OW0	HOH	W	525	-39.430	-3.446	11.094	1.00	31.95
18966	OW0	HOH	W	528	7.785	-9.738	48.207	1.00	33.07
18969	OW0	HOH	W	530	-18.073	12.719	25.918	1.00	36.54
18972	OW0	HOH	W	531	-58.529	-19.023	-2.956	1.00	29.57
18975	OW0	HOH	W	532	-44.578	-42.328	-28.269	1.00	41.03
18978	OW0	HOH	W	534	-62.763	-32.102	31.943	1.00	37.06
18981	OW0	HOH	W	535	-1.636	-9.374	-9.486	1.00	32.15
18984	OW0	HOH	W	536	9.768	15.243	10.622	1.00	38.05
18987	OW0	HOH	W	537	-8.934	-19.171	7.039	1.00	35.97
18990	OW0	HOH	W	538	-33.907	-22.089	-10.376	1.00	31.10
18993	OW0	HOH	W	539	6.905	-6.657	17.277	1.00	31.28
18996	OW0	HOH	W	542	-44.743	-42.956	-23.096	1.00	29.69
18999	OW0	HOH	W	544	-4.504	-16.432	40.724	1.00	33.95
19002	OW0	HOH	W	545	-38.664	-32.741	17.308	1.00	32.11
19005	OW0	HOH	W	546	-67.425	-51.110	-14.488	1.00	35.68
19008	OW0	HOH	W	547	-52.658	-34.447	-22.208	1.00	26.99
19011	OW0	HOH	W	548	-48.176	-25.147	34.605	1.00	35.16
19014	OW0	HOH	W	549	-22.804	20.072	21.180	1.00	45.74
19017	OW0	HOH	W	550	12.080	8.634	36.491	1.00	32.88
19020	OW0	HOH	W	551	-8.841	21.071	11.431	1.00	34.30
19023	OW0	HOH	W	552	-63.675	-49.886	23.656	1.00	38.75
19026	OW0	HOH	W	554	-19.525	-17.148	16.831	1.00	35.38
19029	OW0	HOH	W	555	-59.553	-19.831	-27.686	1.00	26.18
19032	OW0	HOH	W	556	-47.681	-30.942	32.267	1.00	31.60
19035	OW0	HOH	W	558	-2.291	-11.981	0.426	1.00	28.90
19038	OW0	HOH	W	559	-4.750	-15.367	47.709	1.00	39.25
19041	OW0	HOH	W	560	-65.806	-32.169	-3.667	1.00	35.46
19044	OW0	HOH	W	562	-17.437	-10.533	-16.296	1.00	34.42
19047	OW0	HOH	W	564	-33.398	-3.310	17.572	1.00	31.60
19050	OW0	HOH	W	566	-5.896	-7.339	48.765	1.00	32.27
19053	OW0	HOH	W	567	-50.675	-15.097	-4.492	1.00	29.37
19056	OW0	HOH	W	568	-38.944	-33.504	-33.477	1.00	39.95
19059	OW0	HOH	W	571	-14.223	-20.671	12.061	1.00	32.48
19062	OW0	HOH	W	572	-67.268	-47.382	22.282	1.00	50.74
19065	OW0	HOH	W	573	3.281	-17.655	22.834	1.00	34.58
19068	OW0	HOH	W	574	-5.702	14.693	10.132	1.00	32.40
19071	OW0	HOH	W	575	-11.243	14.624	9.771	1.00	37.28
19074	OW0	HOH	W	576	2.749	5.936	3.950	1.00	30.45
19077	OW0	HOH	W	578	-62.203	-16.917	-20.098	1.00	38.72
19080	OW0	HOH	W	580	-12.387	-2.647	44.353	1.00	48.36
19083	OW0	HOH	W	581	-43.752	-10.106	-16.524	1.00	31.54

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
19086	OWO	HOH	W	582	-7.354	-19.038	3.852	1.00	57.83
19089	OWO	HOH	W	583	-64.054	-25.053	1.484	1.00	31.88
19092	OWO	HOH	W	584	-13.768	-25.250	-1.843	1.00	35.26
19095	OWO	HOH	W	585	-8.589	-7.417	45.243	1.00	35.13
19098	OWO	HOH	W	586	11.350	-10.436	43.963	1.00	25.78
19101	OWO	HOH	W	587	10.253	-8.062	47.024	1.00	33.26
19104	OWO	HOH	W	588	-60.492	-35.039	33.564	1.00	30.90
19107	OWO	HOH	W	589	-11.858	-20.603	-1.371	1.00	30.08
19110	OWO	HOH	W	591	-66.898	-33.417	7.201	1.00	31.51
19113	OWO	HOH	W	592	1.391	14.903	29.762	1.00	30.67
19116	OWO	HOH	W	593	-11.800	18.567	3.944	1.00	37.87
19119	OWO	HOH	W	594	-67.323	-40.595	-6.207	1.00	34.96
19122	OWO	HOH	W	595	18.041	-10.017	43.820	1.00	33.21
19125	OWO	HOH	W	596	-59.397	-20.934	0.873	1.00	34.30
19128	OWO	HOH	W	597	-53.886	-53.056	-17.213	1.00	32.38
19131	OWO	HOH	W	598	-5.240	-7.670	-11.610	1.00	35.07
19134	OWO	HOH	W	599	-55.540	-10.508	-17.058	1.00	33.73
19137	OWO	HOH	W	600	-31.472	-52.639	-2.035	1.00	44.20
19140	OWO	HOH	W	601	-1.496	19.752	16.578	1.00	30.16
19143	OWO	HOH	W	602	-51.477	-57.592	-2.784	1.00	37.10
19146	OWO	HOH	W	603	-58.367	-37.864	-24.952	1.00	34.96
19149	OWO	HOH	W	604	9.069	16.102	18.827	1.00	35.39
19152	OWO	HOH	W	605	-45.862	-43.864	23.966	1.00	32.20
19155	OWO	HOH	W	606	-6.133	6.478	41.672	1.00	35.34
19158	OWO	HOH	W	607	-29.917	-23.302	1.823	1.00	39.63
19161	OWO	HOH	W	608	-28.396	-7.050	-19.485	1.00	37.35
19164	OWO	HOH	W	609	17.828	-10.152	38.439	1.00	40.49
19167	OWO	HOH	W	610	-67.104	-46.801	-6.067	1.00	31.67
19170	OWO	HOH	W	611	-57.493	-44.912	-14.700	1.00	47.65
19173	OWO	HOH	W	612	19.616	-6.016	43.565	1.00	34.99
19176	OWO	HOH	W	613	-61.247	-13.332	-12.193	1.00	37.70
19179	OWO	HOH	W	614	-23.821	-35.035	-9.705	1.00	32.77
19182	OWO	HOH	W	615	-46.580	-28.574	26.146	1.00	32.12
19185	OWO	HOH	W	616	16.303	-6.043	32.016	1.00	33.14
19188	OWO	HOH	W	618	-40.197	-31.208	12.876	1.00	35.35
19191	OWO	HOH	W	619	-26.466	-2.444	-17.832	1.00	39.51
19194	OWO	HOH	W	620	12.442	-11.212	25.352	1.00	31.34
19197	OWO	HOH	W	621	-21.038	-23.524	9.080	1.00	34.35
19200	OWO	HOH	W	622	-30.036	-4.851	15.707	1.00	33.39
19203	OWO	HOH	W	623	-35.345	-37.381	11.278	1.00	32.98
19206	OWO	HOH	W	625	11.973	-7.654	12.629	1.00	33.05
19209	OWO	HOH	W	626	-38.060	1.365	3.422	1.00	33.60
19212	OWO	HOH	W	627	-25.998	17.027	16.355	1.00	33.69
19215	OWO	HOH	W	628	16.730	-13.989	38.719	1.00	28.05
19218	OWO	HOH	W	629	1.312	14.758	26.114	1.00	30.40
19221	OWO	HOH	W	630	-31.059	-21.069	6.237	1.00	32.58
19224	OWO	HOH	W	632	-27.067	18.630	9.304	1.00	51.53
19227	OWO	HOH	W	633	4.976	4.236	3.559	1.00	36.16
19230	OWO	HOH	W	634	10.053	-13.365	21.320	1.00	34.67

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
19233	OW0	HOH	W	635	14.582	5.940	33.697	1.00	39.50
19236	OW0	HOH	W	636	-36.322	-6.128	6.265	1.00	32.50
19239	OW0	HOH	W	637	-11.957	-11.265	41.352	1.00	36.22
19242	OW0	HOH	W	638	-34.114	-1.478	-6.927	1.00	57.15
19245	OW0	HOH	W	640	-11.156	-16.215	-12.721	1.00	29.42
19248	OW0	HOH	W	641	-14.161	-8.520	38.924	1.00	37.53
19251	OW0	HOH	W	642	-54.017	-34.214	-29.062	1.00	33.45
19254	OW0	HOH	W	644	-9.639	12.615	22.567	1.00	38.95
19257	OW0	HOH	W	645	-48.284	-23.859	-38.901	1.00	33.57
19260	OW0	HOH	W	646	-29.375	-31.538	-23.871	1.00	35.54
19263	OW0	HOH	W	648	-65.998	-59.323	2.613	1.00	30.37
19266	OW0	HOH	W	649	-26.222	-7.873	19.776	1.00	37.55
19269	OW0	HOH	W	650	-60.832	-25.412	26.455	1.00	35.18
19272	OW0	HOH	W	653	-28.434	-25.889	-10.201	1.00	41.73
19275	OW0	HOH	W	654	-41.584	-48.402	-19.987	1.00	32.92
19278	OW0	HOH	W	655	4.618	13.802	23.941	1.00	40.04
19281	OW0	HOH	W	656	-42.634	-36.879	-39.680	1.00	40.50
19284	OW0	HOH	W	658	-41.097	-8.315	-22.234	1.00	36.77
19287	OW0	HOH	W	659	-36.262	-31.820	-0.233	1.00	36.04
19290	OW0	HOH	W	660	-31.563	-13.279	-27.023	1.00	32.92
19293	OW0	HOH	W	661	-59.872	-21.301	19.380	1.00	42.11
19296	OW0	HOH	W	662	8.769	11.776	3.852	1.00	40.03
19299	OW0	HOH	W	664	-4.846	-20.253	31.952	1.00	37.38
19302	OW0	HOH	W	665	-52.163	-51.481	-6.307	1.00	33.32
19305	OW0	HOH	W	667	-56.461	-45.430	33.446	1.00	33.57
19308	OW0	HOH	W	668	-44.169	-10.849	-12.824	1.00	32.95
19311	OW0	HOH	W	669	-37.021	-35.601	13.584	1.00	35.95
19314	OW0	HOH	W	670	-67.656	-26.521	-19.504	1.00	44.88
19317	OW0	HOH	W	671	-22.630	9.603	-7.429	1.00	35.89
19320	OW0	HOH	W	672	-10.098	22.024	13.804	1.00	33.60
19323	OW0	HOH	W	673	1.206	5.563	1.723	1.00	42.76
19326	OW0	HOH	W	674	-69.116	-49.736	0.535	1.00	34.84
19329	OW0	HOH	W	675	-51.481	-21.919	-35.833	1.00	32.27
19332	OW0	HOH	W	677	-43.934	-29.836	-37.737	1.00	27.30
19335	OW0	HOH	W	678	-66.549	-31.199	-15.761	1.00	34.89
19338	OW0	HOH	W	679	-26.262	-19.785	12.305	1.00	38.53
19341	OW0	HOH	W	680	-20.410	9.369	-11.805	1.00	34.00
19344	OW0	HOH	W	681	-66.724	-30.272	-1.345	1.00	38.95
19347	OW0	HOH	W	682	-8.638	6.754	0.799	1.00	44.52
19350	OW0	HOH	W	683	17.621	5.444	24.172	1.00	30.13
19353	OW0	HOH	W	684	-53.014	-15.222	17.209	1.00	30.83
19356	OW0	HOH	W	685	-47.078	-50.821	-7.867	1.00	37.87
19359	OW0	HOH	W	686	15.304	-7.432	23.090	1.00	35.43
19362	OW0	HOH	W	688	-35.512	-26.803	-9.125	1.00	36.82
19365	OW0	HOH	W	689	-38.836	-18.124	-4.639	1.00	53.40
19368	OW0	HOH	W	690	17.003	3.749	27.769	1.00	36.19
19371	OW0	HOH	W	691	-60.119	-36.090	-24.278	1.00	43.60
19374	OW0	HOH	W	692	-51.050	-56.022	-11.487	1.00	33.02
19377	OW0	HOH	W	693	-36.246	-41.579	19.104	1.00	33.41



# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
19380	OWO	HOH	W	694	-19.897	-4.241	-18.623	1.00	34.79
19383	OWO	HOH	W	695	-10.617	-12.300	16.955	1.00	45.30
19386	OWO	HOH	W	696	-73.005	-47.500	13.394	1.00	37.81
19389	OWO	HOH	W	702	10.017	16.666	8.468	1.00	36.22
19392	OWO	HOH	W	704	-31.147	-2.610	18.119	1.00	54.59
19395	OWO	HOH	W	705	-47.768	-53.036	-16.206	1.00	36.04
19398	OWO	HOH	W	707	-9.074	-15.171	39.874	1.00	36.28
19401	OWO	HOH	W	709	-69.961	-29.222	0.924	1.00	42.01
19404	OWO	HOH	W	712	-17.061	-6.896	36.123	1.00	45.99
19407	OWO	HOH	W	713	-40.722	-46.617	15.983	1.00	40.93
19410	OWO	HOH	W	714	-16.605	-24.960	-4.977	1.00	36.33
19413	OWO	HOH	W	715	-30.994	-0.774	22.714	1.00	34.31
19416	OWO	HOH	W	716	-26.391	22.050	10.789	1.00	39.05
19419	OWO	HOH	W	717	-43.591	-39.821	-0.076	1.00	67.11
19422	OWO	HOH	W	719	-39.138	-11.928	-4.250	1.00	31.47
19425	OWO	HOH	W	720	-43.136	-35.161	27.280	1.00	31.46
19428	OWO	HOH	W	721	-61.123	-19.172	-16.004	1.00	34.80
19431	OWO	HOH	W	722	-23.777	-2.071	20.439	1.00	32.59
19434	OWO	HOH	W	724	18.246	-0.713	27.402	1.00	34.36
19437	OWO	HOH	W	725	-67.358	-33.512	4.810	1.00	37.89
19440	OWO	HOH	W	727	-45.486	-43.267	-30.949	1.00	33.17
19443	OWO	HOH	W	728	15.900	-5.563	24.762	1.00	35.93
19446	OWO	HOH	W	729	-41.068	-34.214	26.029	1.00	49.12
19449	OWO	HOH	W	730	7.567	10.216	43.625	1.00	37.91
19452	OWO	HOH	W	731	-6.278	14.052	17.387	1.00	34.97
19455	OWO	HOH	W	732	-59.030	-18.809	-30.103	1.00	40.61
19458	OWO	HOH	W	733	13.254	10.427	30.892	1.00	37.64
19461	OWO	HOH	W	734	-41.995	-44.138	11.750	1.00	27.03
19464	OWO	HOH	W	735	-64.782	-41.465	-15.022	1.00	39.84
19467	OWO	HOH	W	736	-14.979	10.336	-0.914	1.00	43.58
19470	OWO	HOH	W	737	-28.043	-34.320	-21.765	1.00	37.29
19473	OWO	HOH	W	738	-13.688	-20.369	-10.241	1.00	39.21
19476	OWO	HOH	W	739	-51.892	-46.122	-11.472	1.00	35.05
19479	OWO	HOH	W	740	-4.322	15.825	21.292	1.00	41.38
19482	OWO	HOH	W	741	-30.755	-6.480	-17.423	1.00	35.62
19485	OWO	HOH	W	742	-27.967	-14.179	-19.214	1.00	49.89
19488	OWO	HOH	W	743	-47.006	-47.608	1.873	1.00	42.29
19491	OWO	HOH	W	744	-30.643	-11.702	-25.087	1.00	37.49
19494	OWO	HOH	W	745	-29.059	-35.598	-25.541	1.00	38.24
19497	OWO	HOH	W	747	-8.082	9.647	41.013	1.00	36.41
19500	OWO	HOH	W	748	-32.664	-30.994	9.186	1.00	63.48
19503	OWO	HOH	W	749	10.538	-8.675	19.567	1.00	42.51
19506	OWO	HOH	W	750	-72.547	-36.262	27.156	1.00	36.91
19509	OWO	HOH	W	751	-8.930	-12.405	43.587	1.00	42.37
19512	OWO	HOH	W	752	0.494	17.082	19.139	1.00	38.31
19515	OWO	HOH	W	753	-31.505	13.662	17.292	1.00	60.40
19518	OWO	HOH	W	754	6.603	16.466	19.778	1.00	36.93
19521	OWO	HOH	W	755	-35.166	-28.339	-7.207	1.00	42.29
19524	OWO	HOH	W	756	-19.294	7.363	-7.418	1.00	34.43

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
19527	OW0	HOH	W	757	-54.686	-57.608	16.972	1.00	36.60
19530	OW0	HOH	W	758	-32.044	-52.618	0.457	1.00	38.92
19533	OW0	HOH	W	759	-4.233	20.706	16.194	1.00	39.99
19536	OW0	HOH	W	760	-3.994	-18.564	33.720	1.00	40.93
19539	OW0	HOH	W	761	-32.708	11.632	3.446	1.00	36.04
19542	OW0	HOH	W	762	12.810	-22.865	33.542	1.00	38.80
19545	OW0	HOH	W	763	-56.811	-45.771	-16.961	1.00	43.84
19548	OW0	HOH	W	764	-31.646	-12.047	13.260	1.00	33.74
19551	OW0	HOH	W	765	-55.431	-9.480	-12.229	1.00	38.17
19554	OW0	HOH	W	766	-12.447	10.594	34.748	1.00	39.80
19557	OW0	HOH	W	767	-29.840	-26.591	-23.881	1.00	36.62
19560	OW0	HOH	W	768	13.262	3.019	3.991	1.00	37.73
19563	OW0	HOH	W	769	-66.074	-21.844	-3.360	1.00	36.97
19566	OW0	HOH	W	770	-31.757	4.237	-6.397	1.00	44.01
19569	OW0	HOH	W	771	-35.638	-28.528	-0.284	1.00	40.71
19572	OW0	HOH	W	772	-36.329	-3.327	-7.081	1.00	42.09
19575	OW0	HOH	W	773	10.384	11.173	37.668	1.00	44.23
19578	OW0	HOH	W	774	-55.959	-12.272	-8.510	1.00	38.89
19581	OW0	HOH	W	775	-9.526	19.066	9.679	1.00	37.48
19584	OW0	HOH	W	776	-12.091	13.094	36.356	1.00	83.93
19587	OW0	HOH	W	777	-48.122	-22.033	13.717	1.00	32.16
19590	OW0	HOH	W	778	-29.884	-57.538	-15.106	1.00	37.56
19593	OW0	HOH	W	781	-55.440	-55.656	15.488	1.00	45.33
19596	OW0	HOH	W	782	-77.359	-42.349	2.721	1.00	36.78
19599	OW0	HOH	W	783	-51.682	-54.394	-6.114	1.00	36.80
19602	OW0	HOH	W	784	14.393	9.772	36.079	1.00	46.32
19605	OW0	HOH	W	786	-4.168	8.948	36.783	1.00	38.35
19608	OW0	HOH	W	788	-67.029	-62.944	-2.015	1.00	43.68
19611	OW0	HOH	W	789	-40.428	-9.824	-7.912	1.00	40.49
19614	OW0	HOH	W	790	-62.915	-42.548	-16.630	1.00	38.89
19617	OW0	HOH	W	791	-52.825	-42.089	34.703	1.00	44.91
19620	OW0	HOH	W	792	-37.552	-6.135	-0.749	1.00	40.57
19623	OW0	HOH	W	793	-32.051	-50.026	3.277	1.00	40.84
19626	OW0	HOH	W	794	-61.101	-37.685	-19.278	1.00	33.57
19629	OW0	HOH	W	795	-35.870	4.997	-2.357	1.00	34.64
19632	OW0	HOH	W	796	-48.401	-42.176	29.325	1.00	33.75
19635	OW0	HOH	W	797	-47.950	-22.167	9.426	1.00	43.02
19638	OW0	HOH	W	798	-9.631	12.051	17.952	1.00	44.53
19641	OW0	HOH	W	799	-17.675	-15.179	20.745	1.00	33.06
19644	OW0	HOH	W	800	-43.305	-46.921	22.593	1.00	39.81
19647	OW0	HOH	W	801	-20.782	8.437	-9.449	1.00	42.40
19650	OW0	HOH	W	802	-57.684	-31.986	-30.064	1.00	33.96
19653	OW0	HOH	W	804	-26.942	-23.675	-10.310	1.00	58.56
19656	OW0	HOH	W	805	-14.169	-12.275	-14.305	1.00	37.78
19659	OW0	HOH	W	806	4.512	-10.629	11.073	1.00	62.46
19662	OW0	HOH	W	807	-55.536	-53.490	10.686	1.00	34.19
19665	OW0	HOH	W	808	-29.716	-7.934	-21.962	1.00	46.49
19668	OW0	HOH	W	809	-68.867	-30.200	10.493	1.00	35.43
19671	OW0	HOH	W	810	-37.859	-2.833	1.358	1.00	30.01

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
19674	OW0	HOH	W	811	-5.658	17.637	10.271	1.00	37.75
19677	OW0	HOH	W	812	-35.655	-4.316	-14.578	1.00	45.68
19680	OW0	HOH	W	813	-48.672	-10.144	-11.962	1.00	41.34
19683	OW0	HOH	W	815	-66.302	-28.821	-22.538	1.00	32.85
19686	OW0	HOH	W	817	-19.660	11.882	21.576	1.00	42.70
19689	OW0	HOH	W	818	-35.500	-25.126	-0.426	1.00	40.31
19692	OW0	HOH	W	819	-40.612	-34.307	-39.693	1.00	43.85
19695	OW0	HOH	W	820	18.240	-6.505	37.034	1.00	35.11
19698	OW0	HOH	W	821	-45.574	-24.089	13.762	1.00	45.88
19701	OW0	HOH	W	822	2.636	-18.229	7.809	1.00	37.80
19704	OW0	HOH	W	823	-39.559	-36.000	-33.339	1.00	42.54
19707	OW0	HOH	W	824	-42.762	-50.816	4.232	1.00	40.10
19710	OW0	HOH	W	825	-59.622	-22.613	22.458	1.00	40.70
19713	OW0	HOH	W	826	-3.359	18.940	5.502	1.00	35.51
19716	OW0	HOH	W	827	-13.151	-12.145	31.220	1.00	46.20
19719	OW0	HOH	W	828	16.141	5.856	42.112	1.00	39.02
19722	OW0	HOH	W	829	18.163	-12.576	36.994	1.00	39.33
19725	OW0	HOH	W	830	-57.292	-54.828	6.687	1.00	36.64
19728	OW0	HOH	W	832	-5.079	-16.834	17.316	1.00	36.66
19731	OW0	HOH	W	833	-10.725	-13.524	41.783	1.00	41.27
19734	OW0	HOH	W	834	-82.850	-43.281	-3.974	1.00	68.81
19737	OW0	HOH	W	835	17.484	-2.357	30.637	1.00	40.45
19740	OW0	HOH	W	836	-35.868	-45.327	5.468	1.00	38.20
19743	OW0	HOH	W	837	4.009	-15.974	8.040	1.00	39.43
19746	OW0	HOH	W	838	-39.838	-47.566	9.290	1.00	35.40
19749	OW0	HOH	W	839	-27.605	-30.355	-18.042	1.00	33.99
19752	OW0	HOH	W	840	-28.935	-24.491	-16.081	1.00	45.79
19755	OW0	HOH	W	841	-64.004	-22.823	17.751	1.00	44.21
19758	OW0	HOH	W	842	-47.187	-48.498	20.354	1.00	40.78
19761	OW0	HOH	W	843	5.285	16.794	28.520	1.00	37.70
19764	OW0	HOH	W	844	6.390	-0.377	-6.559	1.00	45.09
19767	OW0	HOH	W	846	0.384	18.462	29.518	1.00	46.71
19770	OW0	HOH	W	847	-41.002	-24.170	-38.432	1.00	37.53
19773	OW0	HOH	W	848	-2.900	-15.615	-5.945	1.00	36.12
19776	OW0	HOH	W	849	-37.122	-47.509	5.891	1.00	44.64
19779	OW0	HOH	W	850	-27.338	-38.389	-19.373	1.00	37.10
19782	OW0	HOH	W	854	-4.183	-16.105	19.886	1.00	38.61
19785	OW0	HOH	W	855	-51.682	-22.616	29.880	1.00	41.30
19788	OW0	HOH	W	856	-37.460	-31.614	14.578	1.00	59.71
19791	OW0	HOH	W	857	-49.160	-25.909	-40.459	1.00	41.14
19794	OW0	HOH	W	858	0.016	7.033	-0.046	1.00	36.24
19797	OW0	HOH	W	859	-59.126	-11.753	-11.012	1.00	36.47
19800	OW0	HOH	W	860	-34.286	1.299	20.047	1.00	40.57
19803	OW0	HOH	W	861	13.242	-7.593	10.337	1.00	71.27
19806	OW0	HOH	W	863	14.746	-9.638	25.820	1.00	40.18
19809	OW0	HOH	W	864	-4.571	-19.731	20.575	1.00	51.81
19812	OW0	HOH	W	865	1.644	-6.935	17.186	1.00	37.29
19815	OW0	HOH	W	866	-66.287	-26.968	-7.564	1.00	44.38
19818	OW0	HOH	W	867	16.948	3.018	35.159	1.00	47.77

## FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
19821	OW0	HOH	W	868	-11.024	-10.624	15.182	1.00	35.33
19824	OW0	HOH	W	869	7.088	4.193	-0.030	1.00	51.08
19827	OW0	HOH	W	870	-7.434	-21.688	3.656	1.00	41.59
19830	OW0	HOH	W	873	-46.613	-22.921	11.534	1.00	33.34
19833	OW0	HOH	W	876	-2.361	11.976	39.041	1.00	36.22
19836	OW0	HOH	W	878	-51.068	-15.457	15.052	1.00	39.60
19839	OW0	HOH	W	879	-54.972	-55.010	-6.490	1.00	30.59
19842	OW0	HOH	W	880	3.628	-9.273	9.225	1.00	40.80
19845	OW0	HOH	W	882	-38.610	-17.831	0.472	1.00	40.04
19848	OW0	HOH	W	883	-68.133	-22.820	-5.238	1.00	36.26
19851	OW0	HOH	W	885	-35.149	-45.201	3.093	1.00	43.85
19854	OW0	HOH	W	886	-30.943	-19.307	-10.012	1.00	37.86
19857	OW0	HOH	W	887	-10.796	13.045	1.516	1.00	43.43
19860	OW0	HOH	W	888	-69.426	-50.123	-13.195	1.00	51.67
19863	OW0	HOH	W	889	-34.703	-36.016	-28.224	1.00	40.05
19866	OW0	HOH	W	890	-37.421	-39.936	27.372	1.00	67.80
19869	OW0	HOH	W	891	1.869	-6.985	49.016	1.00	34.65
19872	OW0	HOH	W	892	-40.199	-9.857	-26.501	1.00	40.03
19875	OW0	HOH	W	893	-16.714	1.738	42.998	1.00	40.48
19878	OW0	HOH	W	895	-36.394	-37.186	23.137	1.00	42.92
19881	OW0	HOH	W	896	-65.078	-27.604	-16.027	1.00	34.82
19884	OW0	HOH	W	897	2.317	3.405	0.582	1.00	41.64
19887	OW0	HOH	W	898	-52.345	-24.555	1.090	1.00	73.50
19890	OW0	HOH	W	899	-64.444	-28.268	-5.710	1.00	43.44
19893	OW0	HOH	W	900	-5.096	10.816	37.919	1.00	39.66
19896	OW0	HOH	W	901	-8.372	-13.870	50.589	1.00	52.33
19899	OW0	HOH	W	903	-74.053	-34.203	8.585	1.00	51.28
19902	OW0	HOH	W	906	0.042	4.179	-1.874	1.00	46.75
19905	OW0	HOH	W	907	17.933	6.336	2.929	1.00	38.77
19908	OW0	HOH	W	908	-41.448	-49.817	-22.321	1.00	47.58
19911	OW0	HOH	W	909	-31.552	-25.040	-9.299	1.00	34.16
19914	OW0	HOH	W	910	-59.315	-53.265	9.414	1.00	41.55
19917	OW0	HOH	W	911	-70.283	-32.756	4.028	1.00	31.41
19920	OW0	HOH	W	912	-34.961	-24.335	-10.428	1.00	33.51
19923	OW0	HOH	W	913	-33.234	-9.985	-27.561	1.00	55.18
19926	OW0	HOH	W	914	-37.711	6.063	0.088	1.00	46.08
19929	OW0	HOH	W	915	-69.174	-42.189	-6.029	1.00	46.43
19932	OW0	HOH	W	916	12.084	17.747	13.015	1.00	41.31
19935	OW0	HOH	W	917	-41.426	-31.339	25.608	1.00	41.89
19938	OW0	HOH	W	918	-38.872	-43.866	-22.854	1.00	39.36
19941	OW0	HOH	W	919	-9.967	-12.524	46.380	1.00	47.84
19944	OW0	HOH	W	920	-30.654	-43.148	-20.731	1.00	44.73
19947	OW0	HOH	W	921	-57.529	-50.581	29.387	1.00	40.94
19950	OW0	HOH	W	922	-68.348	-51.800	-8.628	1.00	33.32
19953	OW0	HOH	W	924	-5.598	2.467	45.208	1.00	60.61
19956	OW0	HOH	W	925	-33.318	-47.199	5.987	1.00	54.17
19959	OW0	HOH	W	926	-39.923	-9.539	-4.203	1.00	42.98
19962	OW0	HOH	W	927	-16.440	-10.663	33.647	1.00	37.94
19965	OW0	HOH	W	928	-35.639	10.921	6.734	1.00	38.25

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
19968	OW0	HOH	W	929	-55.719	-22.820	-33.886	1.00	44.58
19971	OW0	HOH	W	930	-25.078	9.378	34.902	1.00	46.02
19974	OW0	HOH	W	931	17.449	8.156	27.075	1.00	36.23
19977	OW0	HOH	W	932	-29.463	-0.322	-16.097	1.00	46.29
19980	OW0	HOH	W	933	-66.282	-45.104	-8.326	1.00	35.61
19983	OW0	HOH	W	934	14.022	-7.932	19.302	1.00	42.82
19986	OW0	HOH	W	935	-14.742	-1.872	-10.466	1.00	39.42
19989	OW0	HOH	W	937	-40.118	-12.307	-7.157	1.00	40.24
19992	OW0	HOH	W	938	3.747	-18.269	27.316	1.00	36.90
19995	OW0	HOH	W	940	-40.173	-7.196	-10.553	1.00	70.95
19998	OW0	HOH	W	941	-34.965	-26.627	-36.508	1.00	36.90
20001	OW0	HOH	W	942	-69.541	-37.196	33.046	1.00	41.43
20004	OW0	HOH	W	943	-64.583	-18.064	-19.899	1.00	41.08
20007	OW0	HOH	W	944	-34.848	-28.690	8.183	1.00	72.86
20010	OW0	HOH	W	945	-62.341	-24.467	28.579	1.00	46.99
20013	OW0	HOH	W	946	-38.484	-7.648	4.600	1.00	54.11
20016	OW0	HOH	W	947	19.087	-5.770	39.595	1.00	35.81
20019	OW0	HOH	W	948	-63.132	-19.501	10.206	1.00	38.27
20022	OW0	HOH	W	949	-49.477	-53.505	1.187	1.00	40.75
20025	OW0	HOH	W	950	-17.808	4.759	17.118	1.00	35.60
20028	OW0	HOH	W	952	-8.030	-21.650	35.429	1.00	52.22
20031	OW0	HOH	W	953	-39.167	-16.387	-3.125	1.00	45.03
20034	OW0	HOH	W	954	-38.987	1.727	20.771	1.00	38.95
20037	OW0	HOH	W	955	-6.387	14.246	21.047	1.00	34.68
20040	OW0	HOH	W	956	-33.396	8.751	-3.654	1.00	42.65
20043	OW0	HOH	W	957	-24.428	11.316	0.325	1.00	31.05
20046	OW0	HOH	W	958	-7.130	-1.308	-15.391	1.00	52.64
20049	OW0	HOH	W	959	-64.600	-23.243	6.931	1.00	50.93
20052	OW0	HOH	W	960	-32.257	16.537	14.398	1.00	70.89
20055	OW0	HOH	W	961	10.768	2.090	49.006	1.00	49.36
20058	OW0	HOH	W	962	-41.930	-24.941	15.108	1.00	42.31
20061	OW0	HOH	W	963	-46.459	-9.495	-13.435	1.00	42.60
20064	OW0	HOH	W	964	4.118	-19.248	32.272	1.00	30.84
20067	OW0	HOH	W	965	-64.627	-54.933	8.563	1.00	48.19
20070	OW0	HOH	W	966	-31.060	11.642	0.870	1.00	54.05
20073	OW0	HOH	W	967	-52.073	-34.644	-31.083	1.00	40.92
20076	OW0	HOH	W	968	-26.505	-21.583	-5.243	1.00	38.89
20079	OW0	HOH	W	969	-36.071	-7.193	8.555	1.00	36.11
20082	OW0	HOH	W	970	-33.308	-5.852	14.029	1.00	37.98
20085	OW0	HOH	W	971	-45.182	-19.371	-1.636	1.00	43.54
20088	OW0	HOH	W	972	-6.399	14.162	0.218	1.00	36.96
20091	OW0	HOH	W	973	-64.505	-21.347	13.135	1.00	36.45
20094	OW0	HOH	W	974	-3.345	-17.470	36.267	1.00	36.91
20097	OW0	HOH	W	975	-52.237	-26.680	-35.964	1.00	42.41
20100	OW0	HOH	W	976	-73.620	-36.656	14.116	1.00	39.66
20103	OW0	HOH	W	977	12.320	-8.497	17.174	1.00	39.02
20106	OW0	HOH	W	978	-48.653	-46.657	19.852	1.00	43.50
20109	OW0	HOH	W	979	-27.920	-23.231	6.185	1.00	48.95
20112	OW0	HOH	W	980	-17.047	-22.472	-13.450	1.00	39.84

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
20115	OW0	HOH	W	982	-8.008	1.600	45.804	1.00	43.09
20118	OW0	HOH	W	983	-35.197	-46.740	-20.576	1.00	38.94
20121	OW0	HOH	W	987	17.699	-10.934	29.750	1.00	38.39
20124	OW0	HOH	W	988	-14.404	6.071	40.012	1.00	44.29
20127	OW0	HOH	W	989	-73.890	-41.371	-10.051	1.00	58.50
20130	OW0	HOH	W	990	-0.814	21.930	8.967	1.00	36.20
20133	OW0	HOH	W	991	-33.349	-6.552	-18.034	1.00	38.88
20136	OW0	HOH	W	993	9.809	13.396	36.339	1.00	42.08
20139	OW0	HOH	W	994	-59.738	-59.995	31.673	1.00	65.76
20142	OW0	HOH	W	995	-14.680	-4.460	-13.662	1.00	56.29
20145	OW0	HOH	W	996	-42.253	-48.661	15.351	1.00	32.85
20148	OW0	HOH	W	997	-49.843	-43.751	-26.738	1.00	52.96
20151	OW0	HOH	W	998	-76.909	-34.239	11.799	1.00	71.95
20154	OW0	HOH	W	999	-68.992	-24.468	12.625	1.00	50.36
20157	OW0	HOH	W	1000	-56.372	-12.440	-15.144	1.00	41.24
20160	OW0	HOH	W	1001	-12.311	2.465	48.515	1.00	62.66
20163	OW0	HOH	W	1003	-21.100	11.371	23.636	1.00	42.05
20166	OW0	HOH	W	1004	-71.877	-36.106	21.471	1.00	45.79
20169	OW0	HOH	W	1005	-28.931	-16.667	-19.543	1.00	60.88
20172	OW0	HOH	W	1007	-41.789	-28.361	18.044	1.00	40.43
20175	OW0	HOH	W	1008	-55.757	-27.022	-32.832	1.00	43.19
20178	OW0	HOH	W	1009	4.734	3.262	1.002	1.00	36.59
20181	OW0	HOH	W	1010	16.356	-16.668	36.026	1.00	34.31
20184	OW0	HOH	W	1011	2.797	17.917	19.785	1.00	39.05
20187	OW0	HOH	W	1012	-58.303	-22.552	-30.309	1.00	40.43
20190	OW0	HOH	W	1013	-71.948	-42.116	19.372	1.00	41.05
20193	OW0	HOH	W	1014	-60.568	-40.290	-19.285	1.00	43.98
20196	OW0	HOH	W	1015	-57.931	-56.708	5.290	1.00	42.97
20199	OW0	HOH	W	1018	-18.403	4.084	38.629	1.00	42.32
20202	OW0	HOH	W	1019	-7.110	19.249	4.983	1.00	35.74
20205	OW0	HOH	W	1020	4.929	-12.004	13.264	1.00	38.23
20208	OW0	HOH	W	1021	-30.597	-27.789	-32.345	1.00	45.36
20211	OW0	HOH	W	1022	-10.230	-14.044	37.786	1.00	48.03
20214	OW0	HOH	W	1023	-31.665	-7.291	12.543	1.00	40.60
20217	OW0	HOH	W	1024	-36.817	-45.781	1.341	1.00	38.68
20220	OW0	HOH	W	1026	-40.485	-43.095	27.340	1.00	46.74
20223	OW0	HOH	W	1028	-1.383	-2.223	-10.825	1.00	69.68
20226	OW0	HOH	W	1029	-29.143	-2.800	15.173	1.00	46.39
20229	OW0	HOH	W	1031	-38.320	-41.713	20.469	1.00	46.17
20232	OW0	HOH	W	1032	-50.209	-55.615	13.019	1.00	55.75
20235	OW0	HOH	W	1033	-20.663	-33.177	-3.663	1.00	44.36
20238	OW0	HOH	W	1035	-11.639	-16.832	25.766	1.00	44.01
20241	OW0	HOH	W	1036	-56.651	-22.166	22.432	1.00	41.00
20244	OW0	HOH	W	1037	-48.873	-9.925	-9.447	1.00	43.22
20247	OW0	HOH	W	1042	2.952	-9.710	6.976	1.00	43.32
20250	OW0	HOH	W	1045	-38.501	-49.638	13.160	1.00	45.32
20253	OW0	HOH	W	1046	-70.746	-34.091	20.360	1.00	40.13
20256	OW0	HOH	W	1047	-61.836	-19.757	-8.305	1.00	43.54
20259	OW0	HOH	W	1048	-7.818	-5.601	46.908	1.00	46.26

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
20262	OW0	HOH	W1049		-29.710	-7.018	13.925	1.00	33.51
20265	OW0	HOH	W1050		-2.726	13.600	41.159	1.00	45.38
20268	OW0	HOH	W1051		-57.424	-38.776	-7.294	1.00	75.52
20271	OW0	HOH	W1052		-41.023	-13.901	-4.550	1.00	39.16
20274	OW0	HOH	W1053		-56.807	-17.727	-7.304	1.00	39.68
20277	OW0	HOH	W1054		-80.001	-43.121	-10.681	1.00	52.38
20280	OW0	HOH	W1057		15.423	9.831	27.145	1.00	42.46
20283	OW0	HOH	W1058		-57.777	-22.043	5.427	1.00	36.01
20286	OW0	HOH	W1059		14.639	-19.923	34.915	1.00	43.98
20289	OW0	HOH	W1060		-70.489	-50.054	-9.096	1.00	60.78
20292	OW0	HOH	W1062		-1.673	-18.586	-0.450	1.00	39.97
20295	OW0	HOH	W1063		-28.617	-6.872	19.681	1.00	38.22
20298	OW0	HOH	W1064		-3.728	7.260	-3.229	1.00	49.98
20301	OW0	HOH	W1065		-16.890	-15.736	18.418	1.00	47.11
20304	OW0	HOH	W1066		12.762	8.853	6.615	1.00	54.85
20307	OW0	HOH	W1067		-18.810	-7.861	-18.727	1.00	48.56
20310	OW0	HOH	W1068		-48.577	-11.610	-15.975	1.00	44.79
20313	OW0	HOH	W1069		-29.664	-14.893	-27.824	1.00	40.76
20316	OW0	HOH	W1070		-64.771	-20.042	-23.937	1.00	49.48
20319	OW0	HOH	W1071		-30.494	-55.455	-16.807	1.00	46.76
20322	OW0	HOH	W1072		-50.987	-32.240	-30.796	1.00	42.72
20325	OW0	HOH	W1073		-43.511	-48.803	3.062	1.00	53.01
20328	OW0	HOH	W1075		-50.671	-55.168	-8.447	1.00	35.64
20331	OW0	HOH	W1076		-72.402	-39.789	20.321	1.00	53.33
20334	OW0	HOH	W1078		-38.246	7.951	23.844	1.00	37.64
20337	OW0	HOH	W1079		-40.096	-38.367	-32.751	1.00	42.40
20340	OW0	HOH	W1081		-34.771	-37.138	20.454	1.00	46.16
20343	OW0	HOH	W1082		-7.513	-9.275	49.910	1.00	44.31
20346	OW0	HOH	W1083		-12.399	-18.529	-12.082	1.00	39.14
20349	OW0	HOH	W1084		-44.256	-25.571	24.245	1.00	42.11
20352	OW0	HOH	W1085		-58.728	-13.781	-9.049	1.00	38.98
20355	OW0	HOH	W1087		6.362	-15.612	19.655	1.00	38.93
20358	OW0	HOH	W1088		-22.463	9.564	-1.993	1.00	36.61
20361	OW0	HOH	W1089		-14.766	-7.538	41.232	1.00	40.29
20364	OW0	HOH	W1090		-33.993	-7.224	-26.469	1.00	43.07
20367	OW0	HOH	W1091		-52.630	-21.935	0.867	1.00	71.53
20370	OW0	HOH	W1092		-7.979	-0.376	47.755	1.00	47.90
20373	OW0	HOH	W1093		0.535	-20.168	20.581	1.00	41.49
20376	OW0	HOH	W1095		-45.846	-29.828	28.346	1.00	41.50
20379	OW0	HOH	W1096		18.939	3.791	21.696	1.00	44.84
20382	OW0	HOH	W1097		-71.581	-31.266	-9.268	1.00	35.68
20385	OW0	HOH	W1098		-41.976	-24.803	12.426	1.00	49.38
20388	OW0	HOH	W1099		-9.052	-17.943	39.833	1.00	57.55
20391	OW0	HOH	W1100		-29.991	-6.798	17.428	1.00	54.44
20394	OW0	HOH	W1101		19.553	-8.796	41.899	1.00	40.55
20397	OW0	HOH	W1102		16.202	-0.069	-3.821	1.00	50.72
20400	OW0	HOH	W1103		-36.720	-9.647	-0.666	1.00	33.93
20403	OW0	HOH	W1104		-57.895	-57.479	17.618	1.00	43.20
20406	OW0	HOH	W1105		-50.283	-42.052	32.661	1.00	42.12

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
20409	OW0	HOH	W1106		-70.626	-28.266	9.870	1.00	50.61
20412	OW0	HOH	W1107		-3.246	-15.399	-8.434	1.00	45.02
20415	OW0	HOH	W1108		-57.811	-21.137	2.958	1.00	48.65
20418	OW0	HOH	W1109		-73.405	-33.400	-3.509	1.00	38.67
20421	OW0	HOH	W1110		-52.781	-53.042	6.868	1.00	50.55
20424	OW0	HOH	W1111		-7.940	-18.296	18.415	1.00	40.73
20427	OW0	HOH	W1112		-47.285	-24.915	27.137	1.00	48.07
20430	OW0	HOH	W1113		10.881	-4.098	49.833	1.00	39.14
20433	OW0	HOH	W1114		-20.053	14.219	-0.401	1.00	38.53
20436	OW0	HOH	W1115		-67.728	-27.901	0.951	1.00	44.30
20439	OW0	HOH	W1116		-30.075	-17.092	11.627	1.00	46.09
20442	OW0	HOH	W1117		-66.860	-26.265	29.407	1.00	51.18
20445	OW0	HOH	W1118		-70.232	-28.254	12.565	1.00	41.66
20448	OW0	HOH	W1119		-16.219	-22.383	12.934	1.00	48.31
20451	OW0	HOH	W1120		0.633	-20.078	24.274	1.00	47.42
20454	OW0	HOH	W1121		-16.067	-0.211	-14.058	1.00	43.40
20457	OW0	HOH	W1122		-14.610	-4.817	-11.054	1.00	49.17
20460	OW0	HOH	W1123		-7.519	-20.767	28.984	1.00	48.13
20463	OW0	HOH	W1125		8.748	-17.029	27.225	1.00	34.21
20466	OW0	HOH	W1126		-59.717	-52.108	29.125	1.00	51.14
20469	OW0	HOH	W1128		16.740	3.721	30.593	1.00	46.28
20472	OW0	HOH	W1129		-14.916	-14.602	32.920	1.00	46.58
20475	OW0	HOH	W1130		10.652	13.149	5.112	1.00	45.35
20478	OW0	HOH	W1131		6.320	17.862	32.533	1.00	41.63
20481	OW0	HOH	W1132		-3.709	20.457	20.058	1.00	58.14
20484	OW0	HOH	W1134		-17.946	-1.901	40.367	1.00	44.24
20487	OW0	HOH	W1135		-24.254	-4.250	22.226	1.00	46.02
20490	OW0	HOH	W1136		-38.130	-6.373	9.787	1.00	52.32
20493	OW0	HOH	W1137		17.397	7.168	19.700	1.00	32.83
20496	OW0	HOH	W1138		-3.616	-19.603	25.017	1.00	38.54
20499	OW0	HOH	W1139		-73.095	-32.921	6.564	1.00	42.40
20502	OW0	HOH	W1140		-50.465	-45.499	-16.196	1.00	50.42
20505	OW0	HOH	W1143		-2.524	0.614	50.624	1.00	53.50
20508	OW0	HOH	W1144		17.502	-3.624	32.935	1.00	46.30
20511	OW0	HOH	W1145		-27.527	-17.849	-16.495	1.00	42.94
20514	OW0	HOH	W1146		-9.763	21.627	18.817	1.00	40.36
20517	OW0	HOH	W1147		-33.107	-32.960	15.334	1.00	54.05
20520	OW0	HOH	W1148		-83.149	-42.853	-1.227	1.00	44.69
20523	OW0	HOH	W1149		-41.631	-31.292	-37.670	1.00	42.10
20526	OW0	HOH	W1151		-38.032	-22.400	4.550	1.00	35.51
20529	OW0	HOH	W1152		15.172	-7.936	27.597	1.00	53.74
20532	OW0	HOH	W1153		-35.108	-5.397	11.639	1.00	58.93
20535	OW0	HOH	W1154		6.671	15.287	23.808	1.00	47.42
20538	OW0	HOH	W1155		-16.755	-4.125	-11.865	1.00	45.88
20541	OW0	HOH	W1156		-2.619	7.470	38.965	1.00	45.39
20544	OW0	HOH	W1157		-45.599	-53.205	-19.771	1.00	47.88
20547	OW0	HOH	W1158		-66.836	-48.254	30.074	1.00	40.28
20550	OW0	HOH	W1159		-2.890	-1.064	-7.040	1.00	35.35
20553	OW0	HOH	W1160		1.777	17.346	26.771	1.00	50.37



# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
20556	OW0	HOH	W1161		-31.137	-37.150	-25.615	1.00	44.13
20559	OW0	HOH	W1162		-65.698	-22.663	-21.450	1.00	46.48
20562	OW0	HOH	W1163		-24.888	6.422	19.466	1.00	41.96
20565	OW0	HOH	W1164		-12.137	-26.208	4.044	1.00	51.85
20568	OW0	HOH	W1166		-35.483	-39.186	-28.609	1.00	41.16
20571	OW0	HOH	W1168		-25.007	-39.283	-14.140	1.00	44.75
20574	OW0	HOH	W1169		-56.664	-11.772	-12.471	1.00	42.61
20577	OW0	HOH	W1170		-27.525	10.827	-4.639	1.00	74.29
20580	OW0	HOH	W1173		-59.609	-35.406	-29.609	1.00	45.50
20583	OW0	HOH	W1175		-61.201	-17.800	-11.164	1.00	46.58
20586	OW0	HOH	W1176		16.124	-14.528	29.107	1.00	48.06
20589	OW0	HOH	W1177		-43.681	-38.904	27.882	1.00	42.65
20592	OW0	HOH	W1179		-56.571	-24.107	-31.340	1.00	40.76
20595	OW0	HOH	W1180		-9.106	-24.791	4.799	1.00	40.24
20598	OW0	HOH	W1181		-50.980	-52.861	4.706	1.00	45.79
20601	OW0	HOH	W1182		-44.337	-11.461	-23.885	1.00	43.61
20604	OW0	HOH	W1183		-68.687	-28.229	-13.591	1.00	47.38
20607	OW0	HOH	W1184		-58.184	-28.074	-32.301	1.00	46.62
20610	OW0	HOH	W1185		-6.584	16.429	18.312	1.00	44.42
20613	OW0	HOH	W1186		-20.056	-11.895	-18.491	1.00	44.74
20616	OW0	HOH	W1189		-48.919	-10.944	-18.164	1.00	35.64
20619	OW0	HOH	W1191		-52.490	-25.458	-1.457	1.00	77.69
20622	OW0	HOH	W1192		-76.225	-47.338	-6.315	1.00	52.45
20625	OW0	HOH	W1193		-34.593	-18.050	-5.173	1.00	52.58
20628	OW0	HOH	W1196		-70.737	-32.503	7.923	1.00	39.96
20631	OW0	HOH	W1197		-35.994	-1.949	-3.892	1.00	44.29
20634	OW0	HOH	W1198		-48.113	-44.763	21.547	1.00	47.90
20637	OW0	HOH	W1199		15.703	12.364	26.350	1.00	45.16
20640	OW0	HOH	W1200		-52.771	-35.203	-33.616	1.00	41.80
20643	OW0	HOH	W1201		-50.570	-24.251	-0.857	1.00	55.23
20646	OW0	HOH	W1202		-10.899	-3.767	-14.520	1.00	40.03
20649	OW0	HOH	W1203		-21.248	-11.958	28.904	1.00	55.28
20652	OW0	HOH	W1205		-46.662	-48.868	3.997	1.00	61.08
20655	OW0	HOH	W1206		10.386	-19.301	30.868	1.00	43.78
20658	OW0	HOH	W1207		-16.126	-16.382	22.473	1.00	44.98
20661	OW0	HOH	W1208		-14.346	-20.139	-12.831	1.00	57.95
20664	OW0	HOH	W1209		-33.377	-25.865	-7.592	1.00	59.43
20667	OW0	HOH	W1210		-44.423	-31.903	27.798	1.00	58.57
20670	OW0	HOH	W1211		6.181	-6.565	48.760	1.00	47.14
20673	OW0	HOH	W1212		-67.440	-42.606	-8.060	1.00	62.41
20676	OW0	HOH	W1213		-1.372	-20.890	26.602	1.00	37.08
20679	OW0	HOH	W1214		18.017	6.363	40.078	1.00	40.48
20682	OW0	HOH	W1215		-35.852	-47.466	13.332	1.00	51.28
20685	OW0	HOH	W1217		-27.671	6.817	-5.841	1.00	57.98
20688	OW0	HOH	W1218		-18.392	13.878	22.447	1.00	34.32
20691	OW0	HOH	W1219		12.929	-16.692	28.731	1.00	45.08
20694	OW0	HOH	W1220		-73.964	-34.468	12.687	1.00	42.58
20697	OW0	HOH	W1221		-63.408	-39.207	36.175	1.00	46.21
20700	OW0	HOH	W1222		-34.522	-34.404	19.481	1.00	53.41

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
20703	OW0	HOH	W1223		-24.478	-15.270	16.261	1.00	39.52
20706	OW0	HOH	W1224		-25.645	-24.875	6.360	1.00	41.55
20709	OW0	HOH	W1225		-36.770	-6.608	-23.090	1.00	43.22
20712	OW0	HOH	W1226		-31.401	-24.001	-0.369	1.00	43.93
20715	OW0	HOH	W1227		-26.394	-35.078	-2.770	1.00	41.00
20718	OW0	HOH	W1228		-2.737	-18.176	19.705	1.00	59.88
20721	OW0	HOH	W1229		-72.269	-53.221	-4.991	1.00	73.80
20724	OW0	HOH	W1230		-3.407	2.823	-4.500	1.00	36.84
20727	OW0	HOH	W1231		-0.792	-16.881	36.725	1.00	43.29
20730	OW0	HOH	W1232		-59.010	-27.779	28.351	1.00	45.57
20733	OW0	HOH	W1233		-18.727	6.765	-18.782	1.00	48.70
20736	OW0	HOH	W1234		19.698	-3.670	17.499	1.00	46.16
20739	OW0	HOH	W1235		-38.977	-50.811	4.295	1.00	39.88
20742	OW0	HOH	W1236		-37.800	-47.003	-20.180	1.00	41.60
20745	OW0	HOH	W1237		-69.965	-24.328	-10.630	1.00	59.55
20748	OW0	HOH	W1238		-49.493	-50.918	-16.821	1.00	45.36
20751	OW0	HOH	W1239		10.837	-7.555	7.634	1.00	38.50
20754	OW0	HOH	W1240		-54.758	-19.770	18.974	1.00	43.35
20757	OW0	HOH	W1241		-71.917	-45.906	16.673	1.00	40.04
20760	OW0	HOH	W1243		-72.760	-33.044	-10.916	1.00	50.33
20763	OW0	HOH	W1244		-30.151	18.244	14.650	1.00	70.40
20766	OW0	HOH	W1245		-53.030	-17.328	12.346	1.00	43.39
20769	OW0	HOH	W1246		16.409	10.739	16.328	1.00	41.04
20772	OW0	HOH	W1247		8.809	2.812	-2.186	1.00	57.81
20775	OW0	HOH	W1248		-50.003	-37.300	33.441	1.00	88.77
20778	OW0	HOH	W1249		-17.791	12.935	12.675	1.00	87.04
20781	OW0	HOH	W1250		-4.651	4.270	47.868	1.00	50.20
20784	OW0	HOH	W1251		-58.966	-18.968	15.509	1.00	38.27
20787	OW0	HOH	W1252		-65.232	-43.274	-19.409	1.00	44.64
20790	OW0	HOH	W1253		-66.456	-51.699	18.200	1.00	39.06
20793	OW0	HOH	W1254		-27.222	-35.708	-0.364	1.00	44.15
20796	OW0	HOH	W1255		-71.173	-55.007	-6.670	1.00	43.68
20799	OW0	HOH	W1258		-32.274	-40.992	-2.830	1.00	44.49
20802	OW0	HOH	W1259		-75.537	-48.480	4.539	1.00	44.66
20805	OW0	HOH	W1260		-31.689	-56.690	-11.146	1.00	58.40
20808	OW0	HOH	W1261		-15.793	-17.323	14.629	1.00	37.74
20811	OW0	HOH	W1262		1.040	-9.307	-8.956	1.00	56.83
20814	OW0	HOH	W1263		-30.199	-22.245	-9.833	1.00	43.87
20817	OW0	HOH	W1264		1.887	-19.958	29.091	1.00	45.07
20820	OW0	HOH	W1266		-25.175	-32.149	-2.485	1.00	57.62
20823	OW0	HOH	W1268		-71.875	-24.431	-6.772	1.00	47.78
20826	OW0	HOH	W1269		-54.416	-31.197	33.637	1.00	49.62
20829	OW0	HOH	W1270		-73.114	-35.977	-11.735	1.00	63.01
20832	OW0	HOH	W1271		-48.732	-17.912	-2.637	1.00	38.14
20835	OW0	HOH	W1272		14.282	-0.789	0.573	1.00	62.99
20838	OW0	HOH	W1273		18.336	9.548	21.168	1.00	34.07
20841	OW0	HOH	W1274		-11.020	17.182	8.299	1.00	46.72
20844	OW0	HOH	W1275		-56.308	-32.583	34.647	1.00	55.39
20847	OW0	HOH	W1276		-53.059	-6.933	-11.008	1.00	49.54

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
20850	OW0	HOH	W1277		-33.682	1.731	-10.555	1.00	53.85
20853	OW0	HOH	W1278		-14.041	-10.365	-16.079	1.00	48.12
20856	OW0	HOH	W1279		-42.378	-45.923	-20.138	1.00	35.23
20859	OW0	HOH	W1280		12.714	-0.371	3.775	1.00	35.48
20862	OW0	HOH	W1281		12.827	-4.783	-5.925	1.00	56.80
20865	OW0	HOH	W1282		15.546	-10.905	15.275	1.00	60.98
20868	OW0	HOH	W1284		-45.383	-51.845	-16.888	1.00	33.34
20871	OW0	HOH	W1285		-13.613	-16.936	17.499	1.00	79.24
20874	OW0	HOH	W1287		16.482	-8.689	29.618	1.00	37.76
20877	OW0	HOH	W1291		-28.175	-23.749	-13.771	1.00	42.52
20880	OW0	HOH	W1293		-65.329	-52.850	21.012	1.00	56.30
20883	OW0	HOH	W1294		-41.616	-39.694	10.011	1.00	87.08
20886	OW0	HOH	W1295		12.058	13.341	29.858	1.00	46.88
20889	OW0	HOH	W1297		-39.100	5.300	17.170	1.00	42.82
20892	OW0	HOH	W1298		15.979	-4.376	8.803	1.00	53.37
20895	OW0	HOH	W1299		-40.893	-28.377	22.616	1.00	37.82
20898	OW0	HOH	W1301		-9.731	-14.252	53.144	1.00	47.09
20901	OW0	HOH	W1302		-65.772	-24.484	-25.482	1.00	40.45
20904	OW0	HOH	W1303		-38.314	-7.741	-2.664	1.00	48.75
20907	OW0	HOH	W1304		-65.777	-42.463	-12.776	1.00	47.45
20910	OW0	HOH	W1305		-73.581	-35.041	-9.287	1.00	69.68
20913	OW0	HOH	W1307		-33.109	-25.987	-1.041	1.00	51.86
20916	OW0	HOH	W1308		10.009	15.445	32.303	1.00	56.80
20919	OW0	HOH	W1309		15.213	0.213	2.947	1.00	55.22
20922	OW0	HOH	W1310		-39.310	-12.548	4.050	1.00	46.57
20925	OW0	HOH	W1311		-63.711	-29.882	30.883	1.00	44.90
20928	OW0	HOH	W1312		-60.629	-17.328	-17.871	1.00	45.19
20931	O	HOH	W1313		18.096	-17.288	32.008	1.00	43.08
20934	O	HOH	W1314		-0.725	-19.760	18.506	1.00	47.87
20937	O	HOH	W1315		2.784	-17.968	17.062	1.00	41.58
20940	O	HOH	W1316		8.786	-6.266	15.134	1.00	31.36
20943	O	HOH	W1317		13.948	12.635	19.907	1.00	38.11
20946	O	HOH	W1318		-14.806	20.441	21.077	1.00	48.05
20949	O	HOH	W1319		-16.523	8.583	-3.527	1.00	43.38
20952	O	HOH	W1320		-69.923	-46.278	-8.180	1.00	52.94
20955	O	HOH	W1321		3.341	18.468	32.535	1.00	38.33
20958	O	HOH	W1322		-2.204	17.591	30.197	1.00	46.88
20961	O	HOH	W1323		8.952	15.133	34.661	1.00	54.33
20964	O	HOH	W1324		-56.474	-61.843	19.424	1.00	57.03
20967	O	HOH	W1325		-57.814	-56.179	13.495	1.00	42.32
20970	O	HOH	W1326		-6.015	-0.478	-8.037	1.00	43.90
20973	O	HOH	W1327		-6.284	-1.023	-9.908	1.00	35.26
20976	O	HOH	W1328		-7.759	1.172	-9.379	1.00	35.57
20979	O	HOH	W1329		-41.769	-43.019	-27.379	1.00	38.35
20982	O	HOH	W1330		-42.194	-42.123	-31.281	1.00	39.14
20985	O	HOH	W1331		14.488	-2.677	24.360	1.00	5.98
20988	O	HOH	W1332		-34.373	-3.676	5.309	1.00	5.59
20991	O	HOH	W1333		-30.223	-27.633	-17.087	1.00	8.68
20994	O	HOH	W1334		-71.728	-39.096	13.203	1.00	11.55

# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
20997	O	HOH	W1335		-30.338	-43.697	-8.950	1.00	24.11
21000	O	HOH	W1336		-26.758	-41.983	-12.111	1.00	29.90
21003	O	HOH	W1337		-31.181	-43.613	-12.256	1.00	28.94
21006	O	HOH	W1338		10.323	17.960	6.257	1.00	32.75
21009	O	HOH	W1339		-25.949	-43.186	-9.766	1.00	38.58
21012	O	HOH	W1340		-74.247	-42.254	-4.739	1.00	45.45
21015	O	HOH	W1341		-74.625	-45.718	0.029	1.00	42.82
21018	O	HOH	W1342		-63.430	-20.386	-15.195	1.00	37.69
21021	O	HOH	W1343		18.424	-2.159	21.765	1.00	40.03
21024	O	HOH	W1344		-28.087	-22.697	-7.053	1.00	41.76
21027	O	HOH	W1345		-25.654	-39.647	-8.858	1.00	42.51
21030	O	HOH	W1346		-10.757	9.807	29.597	1.00	18.03
21033	O	HOH	W1347		-78.865	-44.013	-1.225	1.00	43.61
21036	O	HOH	W1348		-28.005	-44.403	-15.406	1.00	45.05
21039	O	HOH	W1349		-28.996	-21.253	-13.131	1.00	38.28
21042	O	HOH	W1350		-34.080	-44.458	-2.158	1.00	40.43
21045	O	HOH	W1351		-30.270	-20.427	-22.355	1.00	40.60
21048	O	HOH	W1352		-12.490	-14.016	26.257	1.00	39.34
21051	O	HOH	W1353		-72.331	-28.725	26.203	1.00	39.11
21054	O	HOH	W1354		12.455	-9.862	-2.273	1.00	40.17
21057	O	HOH	W1355		-56.399	-37.983	-34.218	1.00	41.06
21060	O	HOH	W1356		-68.102	-47.191	-15.728	1.00	42.12
21063	O	HOH	W1357		-18.064	-25.313	7.485	1.00	42.37
21066	O	HOH	W1358		-37.955	-6.382	-25.464	1.00	38.45
21069	O	HOH	W1359		-22.184	-20.389	14.547	1.00	42.79
21072	O	HOH	W1360		-12.421	-8.344	45.312	1.00	45.86
21075	O	HOH	W1361		-86.637	-44.414	-1.657	1.00	42.32
21078	O	HOH	W1362		-43.149	-44.187	26.867	1.00	41.21
21081	O	HOH	W1363		-68.844	-54.135	8.237	1.00	42.37
21084	O	HOH	W1364		-23.818	-21.782	-12.741	1.00	40.25
21087	O	HOH	W1365		-30.594	-37.373	11.717	1.00	40.44
21090	O	HOH	W1366		4.521	-11.975	-0.127	1.00	38.84
21093	O	HOH	W1367		-59.011	-30.143	34.591	1.00	42.68
21096	O	HOH	W1368		-29.988	-47.044	-15.081	1.00	39.85
21099	O	HOH	W1369		-48.928	-50.163	22.069	1.00	39.86
21102	O	HOH	W1370		-74.093	-41.494	16.966	1.00	37.82
21105	O	HOH	W1371		-15.795	-0.031	-16.596	1.00	39.99
21108	O	HOH	W1372		-43.819	-56.476	-6.717	1.00	38.97
21111	O	HOH	W1373		-58.181	-8.340	-20.846	1.00	42.09
21114	O	HOH	W1374		-23.487	9.158	-11.308	1.00	37.80
21117	O	HOH	W1375		0.801	9.979	45.346	1.00	39.07
21120	O	HOH	W1376		13.974	12.196	13.994	1.00	41.70
21123	O	HOH	W1377		-38.422	-40.042	-31.486	1.00	44.56
21126	O	HOH	W1378		-63.501	-43.835	-11.853	1.00	38.04
21129	O	HOH	W1379		-51.965	-9.062	-6.971	1.00	40.87
21132	O	HOH	W1380		-16.058	15.884	27.986	1.00	47.35
21135	O	HOH	W1381		-21.824	-24.781	4.373	1.00	40.47
21138	O	HOH	W1382		-45.322	-13.930	-4.317	1.00	42.60
21141	O	HOH	W1383		-25.331	-41.526	-17.322	1.00	47.10

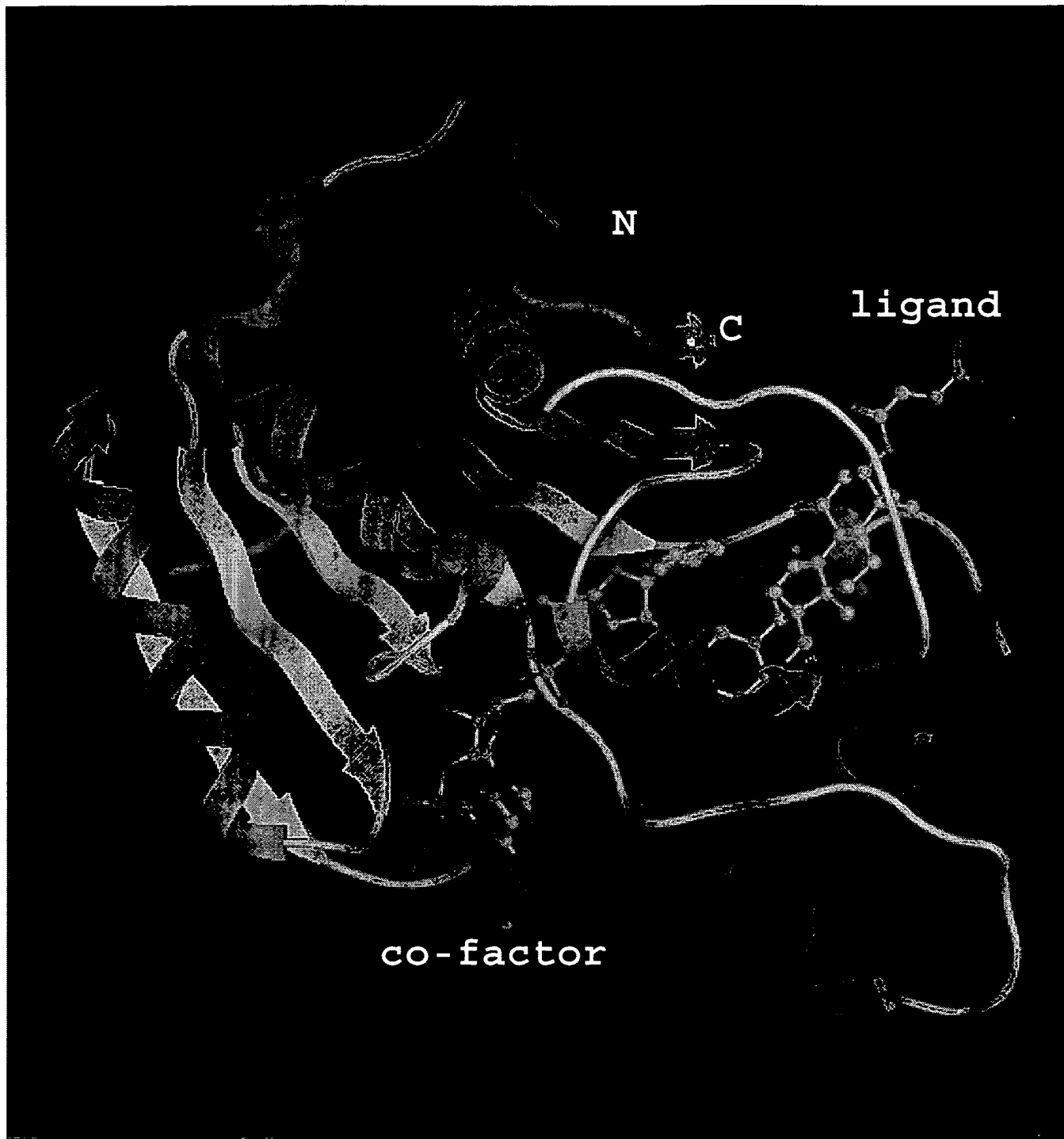
# FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
21144	O	HOH	W1384		-29.594	-10.968	17.972	1.00	41.17
21147	O	HOH	W1385		-50.710	-48.871	28.892	1.00	42.81
21150	O	HOH	W1386		-63.946	-22.712	23.998	1.00	37.65
21153	O	HOH	W1387		-69.553	-53.959	0.118	1.00	41.90
21156	O	HOH	W1388		-28.851	-29.069	-3.979	1.00	44.27
21159	O	HOH	W1389		-48.182	-22.178	23.313	1.00	41.63
21162	O	HOH	W1390		-17.628	10.041	-18.992	1.00	41.83
21165	O	HOH	W1391		-33.865	-16.473	-35.971	1.00	41.00
21168	O	HOH	W1392		10.743	-7.614	-3.480	1.00	42.63
21171	O	HOH	W1393		-22.946	-24.502	0.404	1.00	44.11
21174	O	HOH	W1394		-29.252	-21.552	-17.491	1.00	41.76
21177	O	HOH	W1395		-62.536	-36.646	-21.204	1.00	39.65
21180	O	HOH	W1396		3.638	20.109	21.008	1.00	42.52
21183	O	HOH	W1397		9.649	7.530	46.604	1.00	44.53
21186	O	HOH	W1398		15.051	-7.044	4.413	1.00	41.41
21189	O	HOH	W1399		-67.924	-24.553	-8.393	1.00	41.29
21192	O	HOH	W1400		-67.124	-52.232	-19.913	1.00	42.75
21195	O	HOH	W1401		-28.793	5.301	-15.618	1.00	45.15
21198	O	HOH	W1402		-25.129	-35.296	-19.164	1.00	40.26
21201	O	HOH	W1403		2.859	9.653	-7.062	1.00	44.45
21204	O	HOH	W1404		-73.519	-38.873	25.404	1.00	45.11
21207	O	HOH	W1405		-26.609	-47.583	-11.685	1.00	44.69
21210	O	HOH	W1406		-61.527	-19.034	-25.509	1.00	43.43
21213	O	HOH	W1407		-64.726	-27.112	-29.501	1.00	48.26
21216	O	HOH	W1408		9.240	-10.488	15.070	1.00	41.83
21219	O	HOH	W1409		-33.366	-9.172	-22.210	1.00	40.59
21222	O	HOH	W1410		-29.963	-24.016	-2.756	1.00	42.70
21225	O	HOH	W1411		-37.028	-31.913	19.357	1.00	40.72
21228	O	HOH	W1412		-59.141	-12.954	-19.001	1.00	42.19
21231	O	HOH	W1413		-36.156	-10.186	6.767	1.00	38.39
21234	O	HOH	W1414		-41.516	-50.551	19.356	1.00	46.20
21237	O	HOH	W1415		-2.321	15.372	23.575	1.00	47.07
21240	O	HOH	W1416		-12.119	-4.719	47.509	1.00	42.66
21243	O	HOH	W1417		-9.354	6.417	-16.213	1.00	41.97
21246	O	HOH	W1418		-73.557	-33.299	1.728	1.00	42.41
21249	O	HOH	W1419		-21.337	20.358	28.076	1.00	46.61
21252	O	HOH	W1420		-35.775	-30.515	1.997	1.00	40.56
21255	O	HOH	W1421		-68.477	-20.490	-24.594	1.00	42.08
21258	O	HOH	W1422		-35.441	-52.200	11.972	1.00	45.22
21261	O	HOH	W1423		-67.497	-27.459	-1.749	1.00	43.82
21264	O	HOH	W1424		-20.747	-19.987	-15.392	1.00	43.41
21267	O	HOH	W1425		-58.078	-50.609	-16.710	1.00	47.18
21270	O	HOH	W1426		-1.405	-14.756	-2.162	1.00	39.06
21273	O	HOH	W1427		-18.679	2.686	40.884	1.00	39.91
21276	O	HOH	W1428		-25.966	11.325	-11.442	1.00	43.38
21279	O	HOH	W1429		-41.743	-54.854	2.045	1.00	43.87
21282	O	HOH	W1430		-9.926	-19.720	16.088	1.00	50.72
21285	O	HOH	W1431		8.128	-14.931	16.977	1.00	45.07
21288	O	HOH	W1432		-48.262	-55.165	-8.121	1.00	43.00

### FIGURE 3 (cont.)

A	B	C	D	E	F	G	H	I	J
21291	O	HOH	W1433		-50.106	-57.579	-8.631	1.00	41.39
21294	O	HOH	W1434		-76.001	-35.355	17.245	1.00	44.95
21297	O	HOH	W1435		-30.392	-19.047	-16.185	1.00	37.61
21300	O	HOH	W1436		-31.321	-49.943	-5.443	1.00	37.32

**FIGURE 4**



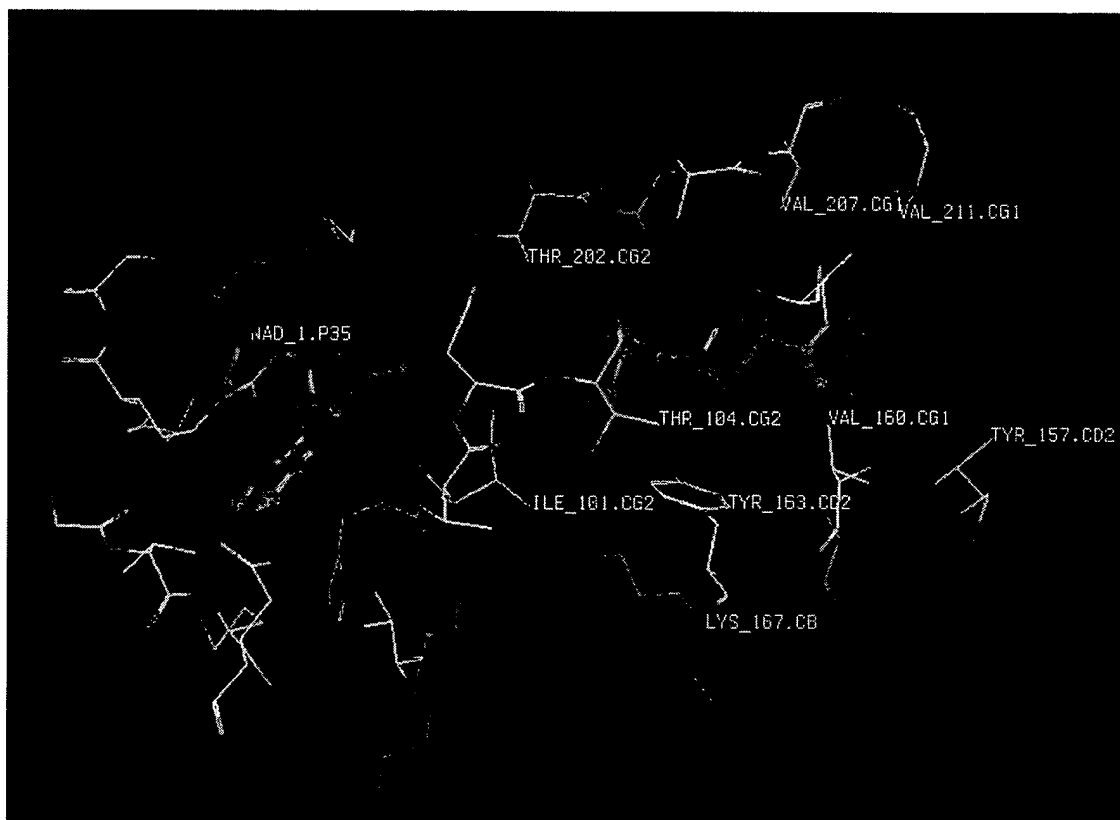
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**FIGURE 5**



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**FIGURE 6**

